```
=> file registry
FILE 'REGISTRY' ENTERED AT 10:07:20 ON 07 DEC 2007
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STRUCTURE FILE UPDATES:     6 DEC 2007  HIGHEST RN 957014-20-9
DICTIONARY FILE UPDATES:    6 DEC 2007  HIGHEST RN 957014-20-9

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TSCA INFORMATION NOW CURRENT THROUGH June 29, 2007

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predicted properties as well as tags indicating availability of
experimental property data in the original document.  For information
on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

=> file zcaplus
FILE 'ZCAPLUS' ENTERED AT 10:07:24 ON 07 DEC 2007
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FILE COVERS 1907 - 7 Dec 2007  VOL 147 ISS 25
FILE LAST UPDATED: 6 Dec 2007  (20071206/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

  This file contains CAS Registry Numbers for easy and accurate
  substance identification.
'OBI' IS DEFAULT SEARCH FIELD FOR 'ZCAPLUS' FILE

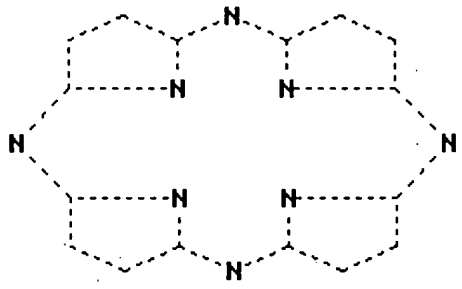
=> d stat que L72
L70          362 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  TAKAKI K?/AU
L71          929 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  YAMASAKI Y?/AU
L72            7 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  L70 AND L71

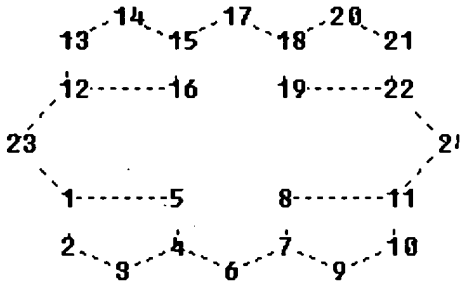

=> d stat que L73
```

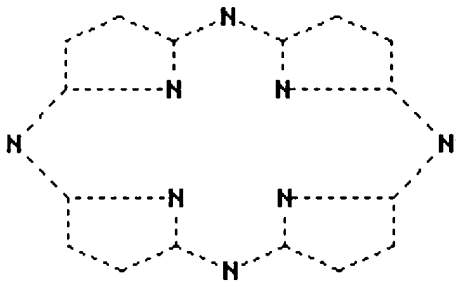
L4 STR

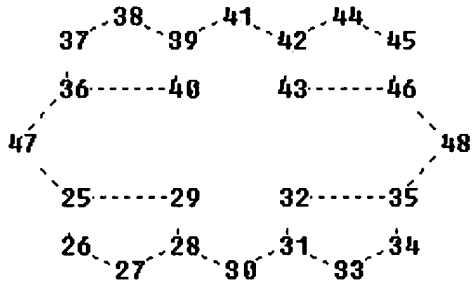
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation:
Uploading L4b.str









ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23
24 25 26 27 28 29 30 31 32 33 34 35 36 37 38 39 40 41 42 43 44
45 46 47 48

ring bonds :
1-2 1-5 1-23 2-3 3-4 4-5 4-6 6-7 7-8 7-9 8-11 9-10 10-11 11-24 12-13
12-16 12-23 13-14 14-15 15-16 15-17 17-18 18-19 18-20 19-22 20-21 21-22
22-24 25-26
25-29 25-47 26-27 27-28 28-29 28-30 30-31 31-32 31-33 32-35 33-34 34-35
35-48 36-37
36-40 36-47 37-38 38-39 39-40 39-41 41-42 42-43 42-44 43-46 44-45 45-46
46-48
exact/norm bonds :
1-2 1-5 1-23 2-3 3-4 4-5 4-6 6-7 7-8 7-9 8-11 9-10 10-11 11-24 12-13
12-16 12-23 13-14 14-15 15-16 15-17 17-18 18-19 18-20 19-22 20-21 21-22
22-24 25-26
25-29 25-47 26-27 27-28 28-29 28-30 30-31 31-32 31-33 32-35 33-34 34-35
35-48 36-37
36-40 36-47 37-38 38-39 39-40 39-41 41-42 42-43 42-44 43-46 44-45 45-46
46-48

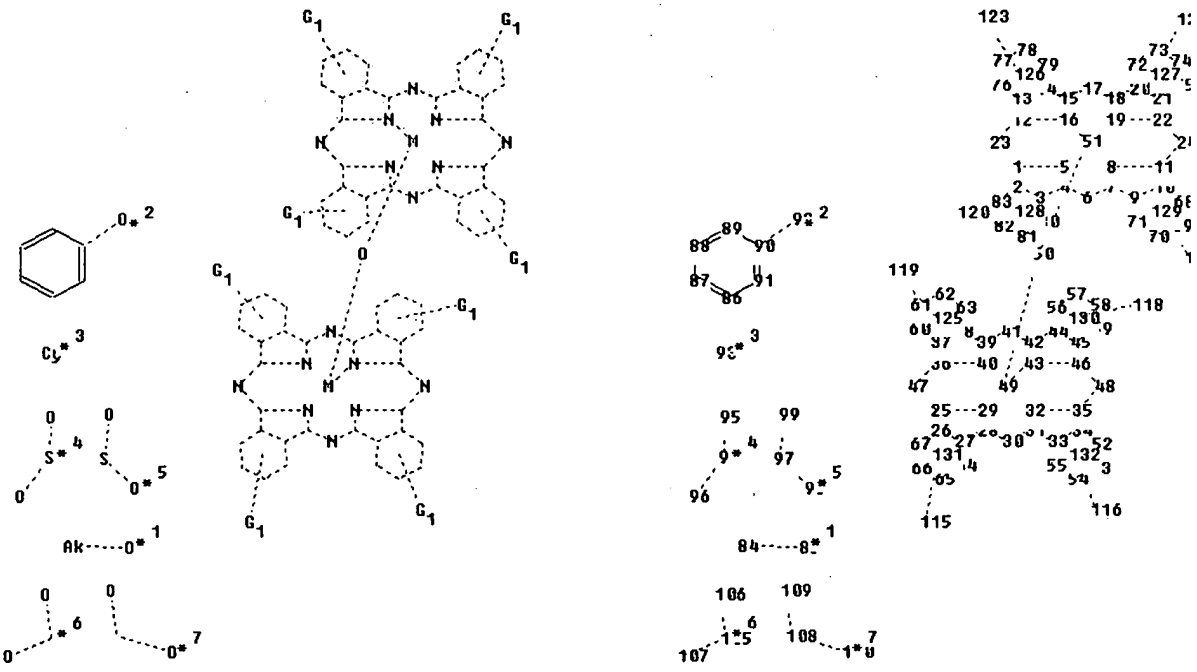
Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom
20:Atom 21:Atom
22:Atom 23:Atom 24:Atom 25:Atom 26:Atom 27:Atom 28:Atom 29:Atom 30:Atom
31:Atom 32:Atom
33:Atom 34:Atom 35:Atom 36:Atom 37:Atom 38:Atom 39:Atom 40:Atom 41:Atom
42:Atom 43:Atom
44:Atom 45:Atom 46:Atom 47:Atom 48:Atom

L5 2661 SEA FILE=REGISTRY SSS FUL L4
L15 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation:
Uploading L15b.str



chain nodes :
50 84 85 92 93 94 95 96 97 98 99 105 106 107 108 109 110 115 116
118 119 120 121 122 123
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23
24 25 26 27 28 29 30 31 32 33 34 35 36 37 38 39 40 41 42 43 44
45 46 47 48
52 53 54 55 56 57 58 59 60 61 62 63 64 65 66 67 68 69 70 71 72
73 74 75
76 77 78 79 80 81 82 83 86 87 88 89 90 91
ring/chain nodes :

49 51
chain bonds :
49-50 50-51 84-85 90-92 94-95 94-96 97-98 97-99 105-106 105-107 108-109
108-110
ring/chain bonds :
16-51 43-49
ring bonds :
1-2 1-5 1-23 2-3 2-83 3-4 3-80 4-5 4-6 6-7 7-8 7-9 8-11 9-10 9-71
10-11 10-68 11-24 12-13 12-16 12-23 13-14 13-76 14-15 14-79 15-16 15-17
17-18 18-19 18-20
19-22 20-21 20-72 21-22 21-75 22-24 25-26 25-29 25-47 26-27 26-67 27-28
27-64 28-29
28-30 30-31 31-32 31-33 32-35 33-34 33-55 34-35 34-52 35-48 36-37 36-40
36-47 37-38
37-60 38-39 38-63 39-40 39-41 41-42 42-43 42-44 43-46 44-45 44-56 45-46
45-59 46-48
52-53 53-54 54-55 56-57 57-58 58-59 60-61 61-62 62-63 64-65 65-66 66-67
68-69 69-70
70-71 72-73 73-74 74-75 76-77 77-78 78-79 80-81 81-82 82-83 86-87 86-91
87-88 88-89
89-90 90-91
exact/norm bonds :
1-2 1-5 1-23 2-3 2-83 3-4 3-80 4-5 4-6 6-7 7-8 7-9 8-11 9-10 9-71
10-11 10-68 11-24 12-13 12-16 12-23 13-14 13-76 14-15 14-79 15-16 15-17
16-51 17-18 18-19
18-20 19-22 20-21 20-72 21-22 21-75 22-24 25-26 25-29 25-47 26-27 26-67
27-28 27-64
28-29 28-30 30-31 31-32 31-33 32-35 33-34 33-55 34-35 34-52 35-48 36-37
36-40 36-47
37-38 37-60 38-39 38-63 39-40 39-41 41-42 42-43 42-44 43-46 43-49 44-45
44-56 45-46
45-59 46-48 49-50 50-51 52-53 53-54 54-55 56-57 57-58 58-59 60-61 61-62
62-63 64-65
65-66 66-67 68-69 69-70 70-71 72-73 73-74 74-75 76-77 77-78 78-79 80-81
81-82 82-83
84-85 90-92 94-95 94-96 97-98 97-99 105-106 105-107 108-109 108-110
normalized bonds :
86-87 86-91 87-88 88-89 89-90 90-91

G1:N,CN,NO2,X,Ak,[*1],[*2],[*3],[*4],[*5],[*6],[*7]

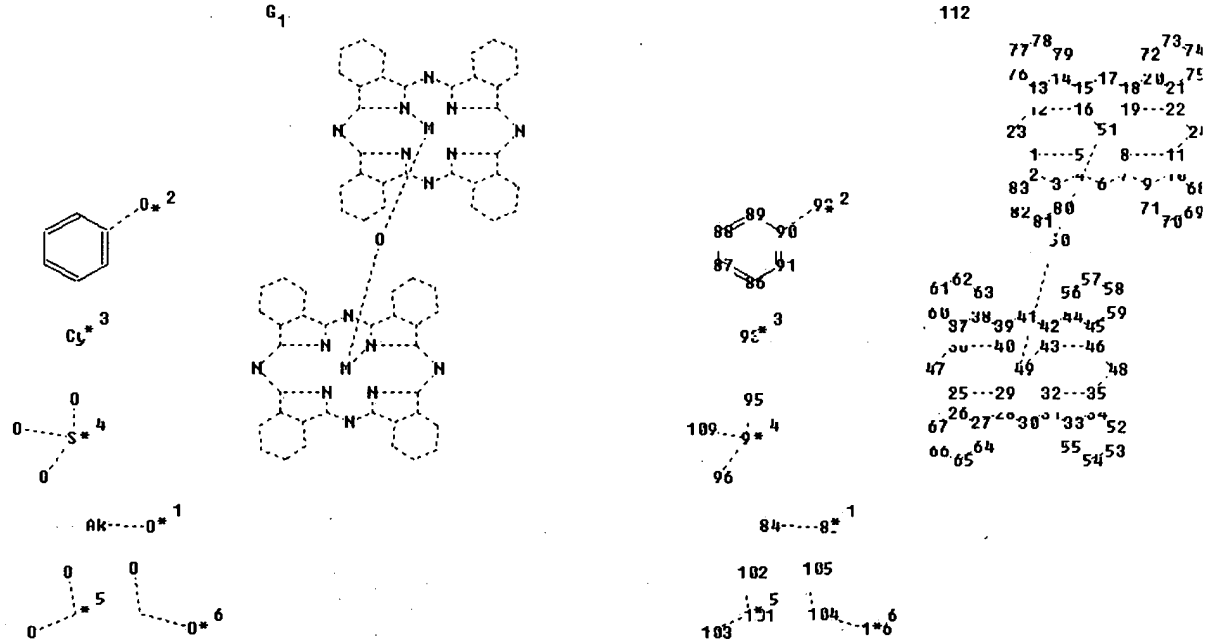
Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom
20:Atom 21:Atom
22:Atom 23:Atom 24:Atom 25:Atom 26:Atom 27:Atom 28:Atom 29:Atom 30:Atom
31:Atom 32:Atom
33:Atom 34:Atom 35:Atom 36:Atom 37:Atom 38:Atom 39:Atom 40:Atom 41:Atom
42:Atom 43:Atom
44:Atom 45:Atom 46:Atom 47:Atom 48:Atom 49:CLASS 50:CLASS 51:CLASS 52:Atom
53:Atom 54:Atom
55:Atom 56:Atom 57:Atom 58:Atom 59:Atom 60:Atom 61:Atom 62:Atom 63:Atom
64:Atom 65:Atom
66:Atom 67:Atom 68:Atom 69:Atom 70:Atom 71:Atom 72:Atom 73:Atom 74:Atom
75:Atom 76:Atom
77:Atom 78:Atom 79:Atom 80:Atom 81:Atom 82:Atom 83:Atom 84:CLASS 85:CLASS
86:Atom 87:Atom
88:Atom 89:Atom 90:Atom 91:Atom 92:CLASS 93:Atom 94:CLASS 95:CLASS 96:CLASS
97:CLASS

98:CLASS 99:CLASS 105:CLASS 106:CLASS 107:CLASS 108:CLASS 109:CLASS
110:CLASS 115:CLASS 116:CLASS
118:CLASS 119:CLASS 120:CLASS 121:CLASS 122:CLASS 123:CLASS 125:Atom
126:Atom 127:Atom
128:Atom 129:Atom 130:Atom 131:Atom 132:Atom
Generic attributes :
93:
Saturation : Unsaturated

L17 58 SEA FILE=REGISTRY SUB=L5 SSS FUL L15
L32 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation:
Uploading L32b.str



chain nodes :
50 84 85 92 93 94 95 96 101 102 103 104 105 106 109 112
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23
24 25 26 27 28 29 30 31 32 33 34 35 36 37 38 39 40 41 42 43 44
45 46 47 48
52 53 54 55 56 57 58 59 60 61 62 63 64 65 66 67 68 69 70 71 72
73 74 75
76 77 78 79 80 81 82 83 86 87 88 89 90 91
ring/chain nodes :
49 51

chain bonds :
49-50 50-51 84-85 90-92 94-95 94-96 94-109 101-102 101-103 104-105 104-106

ring/chain bonds :
16-51 43-49
ring bonds :
1-2 1-5 1-23 2-3 2-83 3-4 3-80 4-5 4-6 6-7 7-8 7-9 8-11 9-10 9-71
10-11 10-68 11-24 12-13 12-16 12-23 13-14 13-76 14-15 14-79 15-16 15-17
17-18 18-19 18-20
19-22 20-21 20-72 21-22 21-75 22-24 25-26 25-29 25-47 26-27 26-67 27-28
27-64 28-29
28-30 30-31 31-32 31-33 32-35 33-34 33-55 34-35 34-52 35-48 36-37 36-40
36-47 37-38
37-60 38-39 38-63 39-40 39-41 41-42 42-43 42-44 43-46 44-45 44-56 45-46
45-59 46-48
52-53 53-54 54-55 56-57 57-58 58-59 60-61 61-62 62-63 64-65 65-66 66-67
68-69 69-70
70-71 72-73 73-74 74-75 76-77 77-78 78-79 80-81 81-82 82-83 86-87 86-91
87-88 88-89
89-90 90-91
exact/norm bonds :
1-2 1-5 1-23 2-3 2-83 3-4 3-80 4-5 4-6 6-7 7-8 7-9 8-11 9-10 9-71
10-11 10-68 11-24 12-13 12-16 12-23 13-14 13-76 14-15 14-79 15-16 15-17
16-51 17-18 18-19
18-20 19-22 20-21 20-72 21-22 21-75 22-24 25-26 25-29 25-47 26-27 26-67
27-28 27-64
28-29 28-30 30-31 31-32 31-33 32-35 33-34 33-55 34-35 34-52 35-48 36-37
36-40 36-47
37-38 37-60 38-39 38-63 39-40 39-41 41-42 42-43 42-44 43-46 43-49 44-45
44-56 45-46
45-59 46-48 49-50 50-51 52-53 53-54 54-55 56-57 57-58 58-59 60-61 61-62
62-63 64-65
65-66 66-67 68-69 69-70 70-71 72-73 73-74 74-75 76-77 77-78 78-79 80-81
81-82 82-83
84-85 90-92 94-95 94-96 94-109 101-102 101-103 104-105 104-106
normalized bonds :
86-87 86-91 87-88 88-89 89-90 90-91

G1:X,Ak,CN,NO2,N,[*1],[*2],[*3],[*4],[*5],[*6]

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom
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33:Atom 34:Atom 35:Atom 36:Atom 37:Atom 38:Atom 39:Atom 40:Atom 41:Atom
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44:Atom 45:Atom 46:Atom 47:Atom 48:Atom 49:CLASS 50:CLASS 51:CLASS 52:Atom
53:Atom 54:Atom
55:Atom 56:Atom 57:Atom 58:Atom 59:Atom 60:Atom 61:Atom 62:Atom 63:Atom
64:Atom 65:Atom
66:Atom 67:Atom 68:Atom 69:Atom 70:Atom 71:Atom 72:Atom 73:Atom 74:Atom
75:Atom 76:Atom
77:Atom 78:Atom 79:Atom 80:Atom 81:Atom 82:Atom 83:Atom 84:CLASS 85:CLASS
86:Atom 87:Atom
88:Atom 89:Atom 90:Atom 91:Atom 92:CLASS 93:Atom 94:CLASS 95:CLASS 96:CLASS
101:CLASS

102:CLASS 103:CLASS 104:CLASS 105:CLASS 106:CLASS 109:CLASS 112:CLASS
Generic attributes :
93:
Saturation : Unsaturated

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L34         154 SEA FILE=REGISTRY SUB=L5 SSS FUL L32
L36           8 SEA FILE=REGISTRY ABB=ON  PLU=ON  L17 AND NC>1
L37           1 SEA FILE=REGISTRY ABB=ON  PLU=ON  L36 AND HYDROXIDE/CNS
L38           1 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  L37
L40           1 SEA FILE=REGISTRY ABB=ON  PLU=ON  L17 AND HYDROXIDE/CNS
L41           6 SEA FILE=REGISTRY ABB=ON  PLU=ON  L34 AND HYDROXIDE/CNS
L42           1 SEA FILE=REGISTRY ABB=ON  PLU=ON  L34 AND SULFATE/CNS
L44         154 SEA FILE=REGISTRY ABB=ON  PLU=ON  L17 OR L34
L46           7 SEA FILE=REGISTRY ABB=ON  PLU=ON  (L40 OR L41 OR L42)
L50           5 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  L46
L57           1 SEA FILE=REGISTRY ABB=ON  PLU=ON  HYDROXIDE/CN
L58           1 SEA FILE=REGISTRY ABB=ON  PLU=ON  SULFATE/CN
L59           1 SEA FILE=REGISTRY ABB=ON  PLU=ON  CHLORIDE/CN
L60           0 SEA FILE=REGISTRY ABB=ON  PLU=ON  H S O/ELF
L61       30961 SEA FILE=REGISTRY ABB=ON  PLU=ON  H O S/ELF
L62       30964 SEA FILE=REGISTRY ABB=ON  PLU=ON  (L57 OR L58 OR L59 OR L60 OR
                L61)
L63          83 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  L44
L64          50 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  L17
L65           4 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  L62 AND (L63 OR L64)
L66           4 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  L65 NOT L50
L67           1 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  L66 AND SULFATE/OBI
L68      581403 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  CHARGE/BI
L69           8 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  (L63 OR L64) AND L68
L70         362 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  TAKAKI K?/AU
L71         929 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  YAMASAKI Y?/AU
L73           3 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  (L70 OR L71) AND (L38 OR L50
                OR L67 OR L69)


=> s L72 or L73
L74           7 L72 OR L73

=> d ibib abs hitind hitstr L74 1-7

L74  ANSWER 1 OF 7  ZCAPLUS  COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER:        2005:1164379  ZCAPLUS  Full-text
DOCUMENT NUMBER:         144:285084
TITLE:                   Synthesis of μ-oxo-bridged hetero-metal
                         phthalocyanine dimer analogues and application for
                         charge generating material in photoreceptor
AUTHOR(S):               Yamasaki, Yasuhiro; Takaki, Kenji
CORPORATE SOURCE:        Research Division, Orient Chemical Industries Limited,
                         8-1 Sanra-Higashi-Machi, Neyagawa, Osaka, 572-8581,
                         Japan
SOURCE:                  Dyes and Pigments (2005), Volume Date 2006, 70(2),
                         105-109
                         CODEN: DYPIDX; ISSN: 0143-7208
PUBLISHER:               Elsevier Ltd.
DOCUMENT TYPE:           Journal
LANGUAGE:                English
```

OTHER SOURCE(S): CASREACT 144:285084

AB The concentrated H_2SO_4 treatment of an equimolar mixture of a halo-(aluminum or gallium) phthalocyanine and an oxo (titanium or vanadium) phthalocyanine followed by treating in a basic solution gives selectively μ-oxo-bridged hetero-metal phthalocyanine dimer (MM'Pc)2O in good yield. This methodol. can also serve μ-oxo-bridged hetero-metal phthalocyanine and naphthalocyanine mixed dimers. The gallium titanium hetero-metal phthalocyanine showed good photoreceptor properties.

CC 78-7 (Inorganic Chemicals and Reactions)
Section cross-reference(s): 74

IT 634179-08-1P 634179-09-2P 634179-10-5P 634179-11-6P 685834-15-5P
685834-17-7P 685834-21-3P 685834-24-6P 685834-28-0P
878274-94-3P 878274-95-4P 878275-02-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of μ-oxo-bridged hetero-metal phthalocyanine and naphthalocyanine dimers)

IT ***878274-94-3P 878274-95-4P 878275-02-6P***
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of μ-oxo-bridged hetero-metal phthalocyanine and naphthalocyanine dimers)

RN 878274-94-3 ZCAPLUS

CN Titanium(1+), μ-oxo[[29H,31H-phthalocyaninato(2-)-κN29,κN30,κN31,κN32]gallium][2,9,16,23-tetrakis(1,1-dimethylethyl)-29H,31H-phthalocyaninato(2-)-κN29,κN30,κN31,κN32]-, hydroxide (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

RN 878274-95-4 ZCAPLUS

CN Titanium(1+), μ-oxo[2,9,16,23-tetrakis(1,1-dimethylethyl)-29H,31H-phthalocyaninato(2-)-κN29,κN30,κN31,κN32][[2,9,16,23-tetrakis(1,1-dimethylethyl)-29H,31H-phthalocyaninato(2-)-κN29,κN30,κN31,κN32]gallium]-, hydroxide (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

RN 878275-02-6 ZCAPLUS

CN Titanium(1+), μ-oxo[[2,9,16,23-tetrakis(1,1-dimethylethyl)-29H,31H-phthalocyaninato(2-)-κN29,κN30,κN31,κN32]gallium][37H,39H-tetranaphtho[2,3-b:2',3'-g:2'',3''-l:2''',3'''-q]porphyrazinato(2-)-κN37,κN38,κN39,κN40]-, hydroxide (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

REFERENCE COUNT: 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L74 ANSWER 2 OF 7 ZCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2004:545745 ZCAPLUS Full-text

DOCUMENT NUMBER: 141:96615

TITLE: Organic electrophotographic photoreceptor

INVENTOR(S): ***Yamasaki, Yasuhiro; Takaki, Kenji***

PATENT ASSIGNEE(S): Orient Chemical Industries, Ltd., Japan

SOURCE: Eur. Pat. Appl., 30 pp.
CODEN: EPXXDW

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1435545	A1	20040707	EP 2004-50	20040105
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
JP 2004212725	A	20040729	JP 2003-523	20030106
US 2004146793	A1	20040729	US 2004-750828	20040105
US 7163772	B2	20070116		
KR 2004063813	A	20040714	KR 2004-546	20040106

PRIORITY APPLN. INFO.: JP 2003-523 A 20030106
OTHER SOURCE(S): MARPAT 141:96615

AB The present invention provides an organic electrophotog. photoreceptor having a conductive substrate and a photosensitive layer laid on the conductive substrate, wherein the photosensitive layer contains at least one μ-oxo bridged heterometal compound as a charge generating material. The organic electrophotog. photoreceptor has high photo-sensitivity, high stability, excellent durability on sensitivity and on elec. potential, and has excellent organic photoconductive property.

IC ICM G03G005-06
ICS C09B067-22; C09B067-00; C09B047-08; C07D487-22; C07D259-00; C07D209-00
CC 74-3 (Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes)
REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L74 ANSWER 3 OF 7 ZCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:386613 ZCAPLUS Full-text
DOCUMENT NUMBER: 140:398881
TITLE: Selective preparation of μ-oxo bridged heterobimetallic dinuclear naphthalocyanine and phthalocyanine compounds
INVENTOR(S): ***Yamasaki, Yasuhiro; Takaki, Kenji***
PATENT ASSIGNEE(S): Orient Chemical Industries, Ltd., Japan
SOURCE: Eur. Pat. Appl., 35 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1418207	A1	20040512	EP 2003-25734	20031110
EP 1418207	B1	20070530		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
JP 2004155996	A	20040603	JP 2002-325347	20021108
US 2004091742	A1	20040513	US 2003-701610	20031106
US 7087747	B2	20060808		

PRIORITY APPLN. INFO.: JP 2002-325347 A 20021108
OTHER SOURCE(S): MARPAT 140:398881

AB An object of the present invention is to provide a new μ-oxo bridged heterometal compound, which can make photo-functional materials having diversified properties, and a production method such that the μ-oxo bridged heterometal compound is obtained simply, selectively and with high yield. The present invention provides μ-oxo bridged heterometal compds., NcM1-O-M2Nc,

PcM1-O-M2Nc and NcM1-O-M2Pc wherein H2Nc represents naphthalocyanine, H2Pc represents phthalocyanine, M1 represents a metal atom (such as Al or Ga) which is able to have a valence of up to three, and M2 represents a metal atom (such as Ti or V) which is able to have a valence of four or five. Thus, [NcGa-μ-O-TiPc](OH) was prepared in 64% yield from chlorogallium naphthalocyanine [ClGaNc] and titanyl phthalocyanine [O:TiPc].

IC ICM C09B067-22
ICS C09B067-00; G03G005-06; C09B047-08; C07D487-22; C07D259-00; C07D209-00

CC 78-7 (Inorganic Chemicals and Reactions)

IT 7429-90-5DP, Aluminum, heterobimetallic naphthalocyanine/phthalocyanine complexes 7440-32-6DP, Titanium, heterobimetallic naphthalocyanine/phthalocyanine complexes 7440-55-3DP, Gallium, heterobimetallic naphthalocyanine/phthalocyanine complexes 7440-62-2DP, Vanadium, heterobimetallic naphthalocyanine/phthalocyanine complexes 685834-15-5P 685834-17-7P 685834-21-3P 685834-23-5P 685834-24-6P 685834-26-8P 685834-28-0P ***686290-60-8P***
RL: SPN (Synthetic preparation); PREP (Preparation)
(selective preparation of μ-oxo bridged heterobimetallic dinuclear naphthalocyanine and phthalocyanine complexes)

IT ***686290-60-8P***
RL: SPN (Synthetic preparation); PREP (Preparation)
(selective preparation of μ-oxo bridged heterobimetallic dinuclear naphthalocyanine and phthalocyanine complexes)

RN 686290-60-8 ZCAPLUS

CN Titanium(1+), μ-oxo[[C,C,C,C-tetrakis(1,1-dimethylethyl)-29H,31H-phthalocyaninato(2-)-κN29,κN30,κN31,κN32]gallium][37H,39H-tetranaphtho[2,3-b:2',3'-g:2'',3''-l:2''',3'''-q]porphyrazinato(2-)-κN37,κN38,κN39,κN40]-, hydroxide (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
REFERENCE COUNT: 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L74 ANSWER 4 OF 7 ZCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2003:991587 ZCAPLUS Full-text
DOCUMENT NUMBER: 140:28629
TITLE: μ-Oxo crosslinked dissimilar metal phthalocyanine compound and process for selectively producing the same
INVENTOR(S): ***Takaki, Kenji; Yamasaki, Yasuhiro***
PATENT ASSIGNEE(S): Orient Chemical Industries, Ltd., Japan
SOURCE: PCT Int. Appl., 41 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003104334	A1	20031218	WO 2003-JP7240	20030609
W: JP, KR, US				
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR				
EP 1514904	A1	20050316	EP 2003-730862	20030609
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, FI, RO, CY, TR, BG, CZ, EE, HU, SK				

US 2006020129 A1 20060126 US 2004-516884 20041203
PRIORITY APPLN. INFO.: JP 2002-168580 A 20020610
WO 2003-JP7240 W 20030609

OTHER SOURCE(S): MARPAT 140:28629

AB The present invention relates to a novel μ-oxo crosslinked dissimilar metal phthalocyanine compound useful as a ***charge*** generating material and a process for selectively producing the μ-oxo crosslinked dissimilar metal phthalocyanine compound in a simple manner with high yield. This μ-oxo crosslinked dissimilar metal phthalocyanine compound comprises a metal phthalocyanine containing central metal M1 and a metal phthalocyanine containing central metal M2, the central metals M1 and M2 oxo crosslinked to each other. Thus, 0.010 mol chlorogallium phthalocyanine obtained from phthalonitrile and gallium trichloride and 0.010 mol titanyl phthalocyanine obtained from phthalonitrile and titanium tetrachloride were reacted in concentrate H2SO4 and washed with water and further with aqueous ammonia to give μ-oxo crosslinked dissimilar metal phthalocyanine with yield 91.0%.

IC ICM C09B047-12
ICS C09B047-067; C09B047-08; C07D487-22; G03G005-06

CC 41-7 (Dyes, Organic Pigments, Fluorescent Brighteners, and Photographic Sensitizers)
Section cross-reference(s): 74

ST oxo crosslinked dissimilar metal phthalocyanine selective prepn; chlorogallium phthalocyanine titanyl phthalocyanine dimer ***charge*** generating material prepn

IT 634179-07-0P 634179-08-1P 634179-09-2P 634179-10-5P 634179-11-6P ***634179-47-8P 634179-48-9P***
RL: IMF (Industrial manufacture); PREP (Preparation)
(preparation of μ-oxo crosslinked dissimilar metal phthalocyanine compds.)

IT ***634179-47-8P 634179-48-9P***
RL: IMF (Industrial manufacture); PREP (Preparation)
(preparation of μ-oxo crosslinked dissimilar metal phthalocyanine compds.)

RN 634179-47-8 ZCAPLUS

CN Titanium(1+), μ-oxo[[29H,31H-phthalocyaninato(2-)-κN29,κN30,κN31,κN32]gallium][C,C,C,C-tetrakis(1,1-dimethylethyl)-29H,31H-phthalocyaninato(2-)-κN29,κN30,κN31,κN32]-, hydroxide (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

RN 634179-48-9 ZCAPLUS

CN Titanium(1+), μ-oxo[C,C,C,C-tetrakis(1,1-dimethylethyl)-29H,31H-phthalocyaninato(2-)-κN29,κN30,κN31,κN32][[C,C,C,C-tetrakis(1,1-dimethylethyl)-29H,31H-phthalocyaninato(2-)-κN29,κN30,κN31,κN32]gallium]-, hydroxide (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L74 ANSWER 5 OF 7 ZCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2000:367072 ZCAPLUS Full-text
DOCUMENT NUMBER: 133:18773
TITLE: Oxoaluminum/gallium phthalocyanine dimers
INVENTOR(S): ***Yamasaki, Yasuhiro; Takaki, Kenji;*** Kuroda, Kazuyoshi
PATENT ASSIGNEE(S): Orient Chemical Industries, Ltd., Japan

SOURCE: Eur. Pat. Appl., 23 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1004634	A2	20000531	EP 1999-123213	19991125
EP 1004634	A3	20020306		
EP 1004634	B1	20031008		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
US 6093514	A	20000725	US 1999-444697	19991124
JP 2000219817	A	20000808	JP 1999-334128	19991125

PRIORITY APPLN. INFO.: JP 1998-335729 A 19981126

AB The μ-oxoaluminum/gallium phthalocyanine dimers and their mixed crystals are suitable as a charge generating material for an organic photoconductive material, such as an electrophotog. photoreceptor. Thus, hydrolyzing a mixture of 0.01 mol chlorogallium phthalocyanine and 0.01 mol. chloroaluminum phthalocyanine with concentrate H2SO4 followed by dehydrating the resulting hydroxymetal phthalocyanine mixture gave an μ-oxo- aluminum/gallium phthalocyanine dimer.

IC ICM C09B067-22
ICS C09B047-04; G03G005-06

CC 41-7 (Dyes, Organic Pigments, Fluorescent Brighteners, and Photographic Sensitizers)
Section cross-reference(s): 74

L74 ANSWER 6 OF 7 ZCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1999:815646 ZCAPLUS Full-text
DOCUMENT NUMBER: 132:144318
TITLE: μ-Oxo-bridged type aluminum and gallium phthalocyanine dimer - Synthesis, polymorphs and its primary evaluation as an electrophotographic receptor
AUTHOR(S): ***Yamasaki, Yasuhiro; Takaki, Kenji;*** Kuroda, Kazuyoshi
CORPORATE SOURCE: 3rd R & D Center, R & D Department, Orient Chemical Industries, Ltd., Neyagawa-shi, 572-8581, Japan
SOURCE: Nippon Kagaku Kaishi (1999), (12), 841-845
CODEN: NKAKB8; ISSN: 0369-4577
PUBLISHER: Nippon Kagakkai
DOCUMENT TYPE: Journal
LANGUAGE: Japanese

AB We already found and reported that the specific polymorphs of μ-oxo-aluminum phthalocyanine dimer and μ-oxo-gallium phthalocyanine dimer have fairly good characteristics as the electrophotog. receptor. In connection with our ongoing works on this field, we are interested in the synthesis of μ-oxo-bridged dimers of diverse metal phthalocyanines for pursuing various charge generating materials in electrophotog. receptors. We report here the results of studies on the polymorphs of the titled phthalocyanine dimer, ie. μ-oxo-bridged between aluminum and gallium phthalocyanine dimer, and their primary electrophotog. evaluation.

CC 74-3 (Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes)
Section cross-reference(s): 29, 75, 78

L74 ANSWER 7 OF 7 ZCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1997:804467 ZCAPLUS Full-text
DOCUMENT NUMBER: 128:83612
TITLE: Synthesis of new polymorphs of μ-oxo-metal(III) phthalocyanine dimers and their photoconductive properties
AUTHOR(S): ***Yamasaki, Yasuhiro***; Kuroda, Kazuyoshi; ***Takaki, Kenji***
CORPORATE SOURCE: I-2 Group, R & D Dep., Orient Chem. Industries, Ltd., Osaka, 572, Japan
SOURCE: Nippon Kagaku Kaishi (1997), (12), 887-898
CODEN: NKAKB8; ISSN: 0369-4577
PUBLISHER: Nippon Kagakkai
DOCUMENT TYPE: Journal
LANGUAGE: Japanese
AB [MPc]2O (M = Al, Ga; H2Pc = phthalocyanine) were prepared and studied their polymorphs through x-ray diffraction anal. [MPc]2O have several polymorphs, but one of the target compds., that is [InPc]2O, could not be synthesized because InPcCl was easily hydrolyzed through acid-pasting treatment procedure to give metal-free phthalocyanine. The characterization of these compds. by the several chemical anal. methods was satisfied for the target mols. and the FD-Mass anal. distinguished clearly between the hydroxymetal phthalocyanine and the corresponding phthalocyanine dimer. The authors also studied their photoconductive properties on the bilayer photoreceptor consisted of the above phthalocyanine dimer as the charge generating material. The specific polymorphos of [AlPc]2O-II have good spectral response of the photosensitivity in the shorter wavelength, and the [GaPc]2O-G has a fairly high photosensitivity in the wavelength region of laser diode light wavelength, compared with the common phthalocyanine photoreceptors.
CC 78-7 (Inorganic Chemicals and Reactions)
Section cross-reference(s): 72, 73, 74

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DICTIONARY FILE UPDATES:   6 DEC 2007  HIGHEST RN 957014-20-9

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FILE LAST UPDATED: 6 Dec 2007  (20071206/ED)

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=> d stat que L38
L4              STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY -  AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation:
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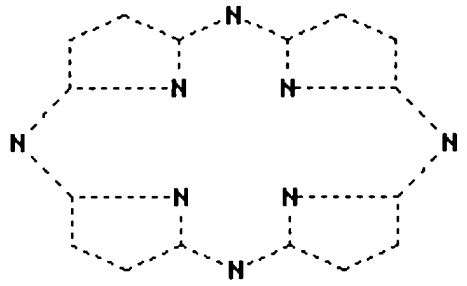

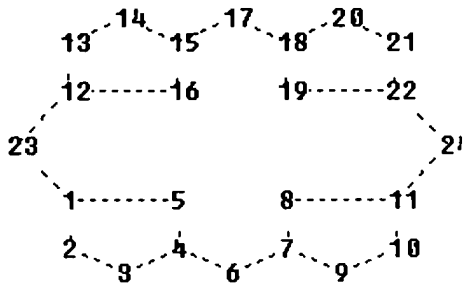

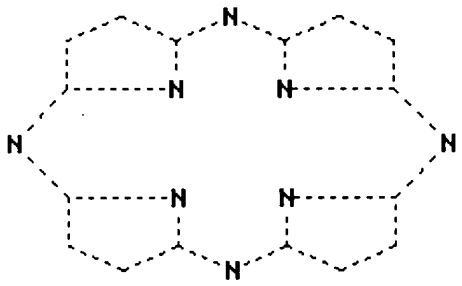

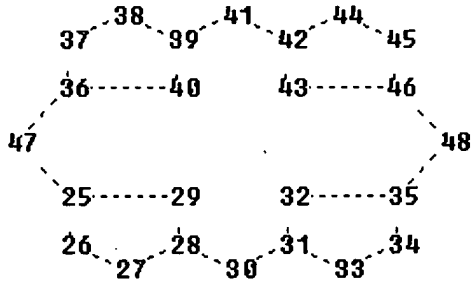

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24 25 26 27 28 29 30 31 32 33 34 35 36 37 38 39 40 41 42 43 44
45 46 47 48

ring bonds :
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12-16 12-23 13-14 14-15 15-16 15-17 17-18 18-19 18-20 19-22 20-21 21-22
22-24 25-26
25-29 25-47 26-27 27-28 28-29 28-30 30-31 31-32 31-33 32-35 33-34 34-35
35-48 36-37
36-40 36-47 37-38 38-39 39-40 39-41 41-42 42-43 42-44 43-46 44-45 45-46
46-48
exact/norm bonds :
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12-16 12-23 13-14 14-15 15-16 15-17 17-18 18-19 18-20 19-22 20-21 21-22
22-24 25-26
25-29 25-47 26-27 27-28 28-29 28-30 30-31 31-32 31-33 32-35 33-34 34-35
35-48 36-37
36-40 36-47 37-38 38-39 39-40 39-41 41-42 42-43 42-44 43-46 44-45 45-46
46-48

Match level :
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11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom
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33:Atom 34:Atom 35:Atom 36:Atom 37:Atom 38:Atom 39:Atom 40:Atom 41:Atom
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44:Atom 45:Atom 46:Atom 47:Atom 48:Atom

L5 2661 SEA FILE=REGISTRY SSS FUL L4
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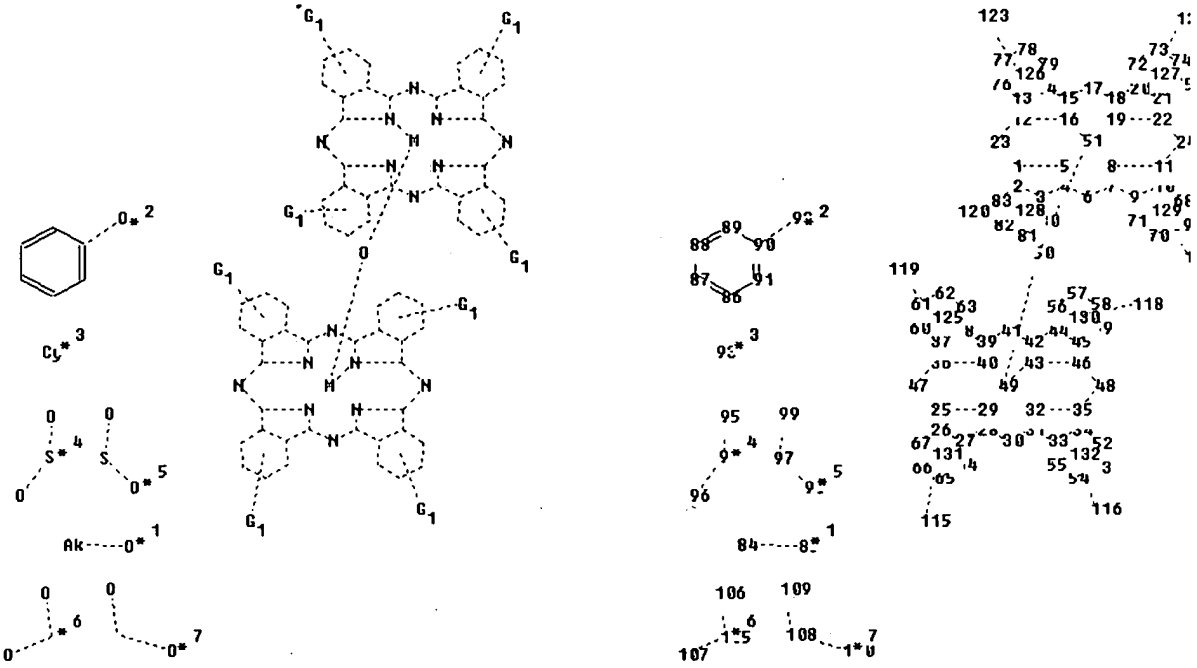

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118 119 120 121 122 123
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24 25 26 27 28 29 30 31 32 33 34 35 36 37 38 39 40 41 42 43 44
45 46 47 48
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73 74 75
76 77 78 79 80 81 82 83 86 87 88 89 90 91
ring/chain nodes :
49 51
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108-110
ring/chain bonds :

16-51 43-49
ring bonds :
1-2 1-5 1-23 2-3 2-83 3-4 3-80 4-5 4-6 6-7 7-8 7-9 8-11 9-10 9-71
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89-90 90-91
exact/norm bonds :
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84-85 90-92 94-95 94-96 97-98 97-99 105-106 105-107 108-109 108-110
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Match level :
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Saturation : Unsaturated

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=> d stat que L50
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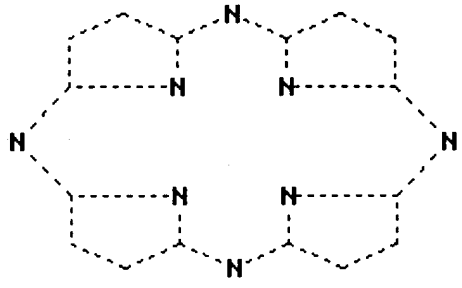
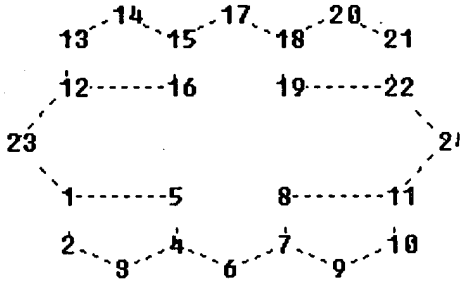
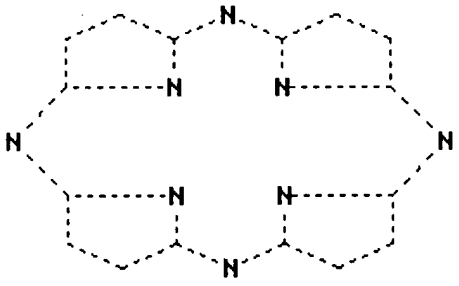
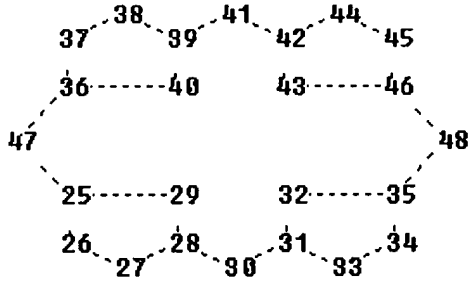








ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23
24 25 26 27 28 29 30 31 32 33 34 35 36 37 38 39 40 41 42 43 44
45 46 47 48

ring bonds :
1-2 1-5 1-23 2-3 3-4 4-5 4-6 6-7 7-8 7-9 8-11 9-10 10-11 11-24 12-13
12-16 12-23 13-14 14-15 15-16 15-17 17-18 18-19 18-20 19-22 20-21 21-22
22-24 25-26

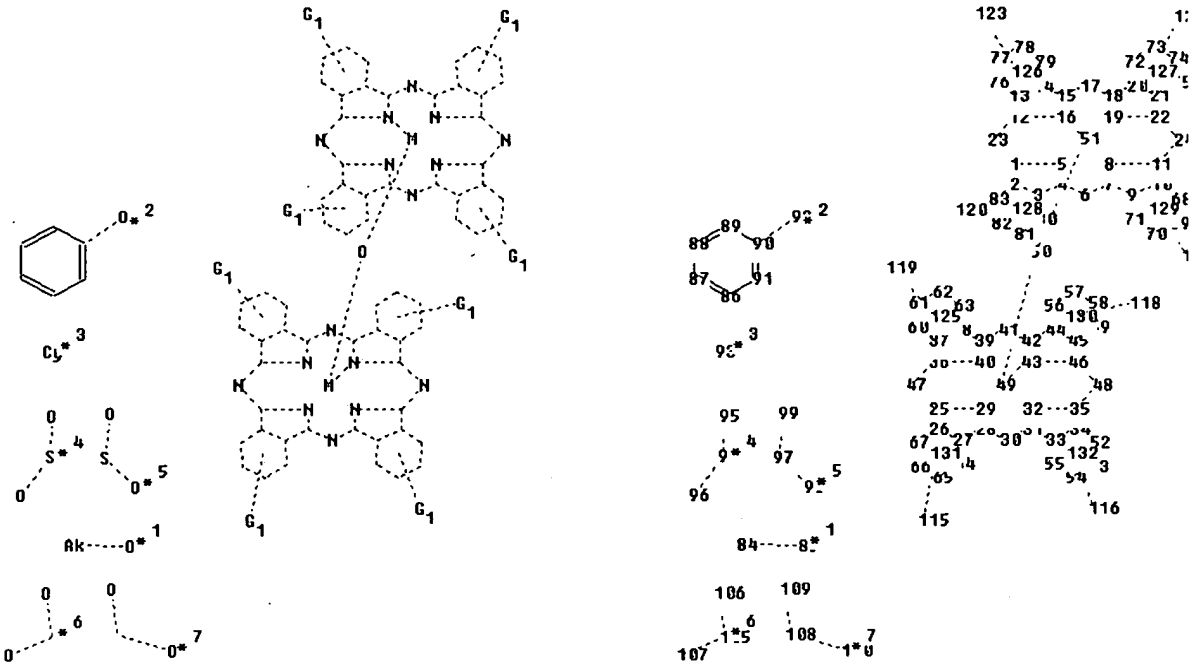
25-29 25-47 26-27 27-28 28-29 28-30 30-31 31-32 31-33 32-35 33-34 34-35
35-48 36-37
36-40 36-47 37-38 38-39 39-40 39-41 41-42 42-43 42-44 43-46 44-45 45-46
46-48
exact/norm bonds :
1-2 1-5 1-23 2-3 3-4 4-5 4-6 6-7 7-8 7-9 8-11 9-10 10-11 11-24 12-13
12-16 12-23 13-14 14-15 15-16 15-17 17-18 18-19 18-20 19-22 20-21 21-22
22-24 25-26
25-29 25-47 26-27 27-28 28-29 28-30 30-31 31-32 31-33 32-35 33-34 34-35
35-48 36-37
36-40 36-47 37-38 38-39 39-40 39-41 41-42 42-43 42-44 43-46 44-45 45-46
46-48

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom
20:Atom 21:Atom
22:Atom 23:Atom 24:Atom 25:Atom 26:Atom 27:Atom 28:Atom 29:Atom 30:Atom
31:Atom 32:Atom
33:Atom 34:Atom 35:Atom 36:Atom 37:Atom 38:Atom 39:Atom 40:Atom 41:Atom
42:Atom 43:Atom
44:Atom 45:Atom 46:Atom 47:Atom 48:Atom

L5 2661 SEA FILE=REGISTRY SSS FUL L4
L15 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation:
Uploading L15b.str



chain nodes :
50 84 85 92 93 94 95 96 97 98 99 105 106 107 108 109 110 115 116
118 119 120 121 122 123
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23
24 25 26 27 28 29 30 31 32 33 34 35 36 37 38 39 40 41 42 43 44
45 46 47 48
52 53 54 55 56 57 58 59 60 61 62 63 64 65 66 67 68 69 70 71 72
73 74 75
76 77 78 79 80 81 82 83 86 87 88 89 90 91
ring/chain nodes :
49 51
chain bonds :
49-50 50-51 84-85 90-92 94-95 94-96 97-98 97-99 105-106 105-107 108-109
108-110
ring/chain bonds :
16-51 43-49
ring bonds :
1-2 1-5 1-23 2-3 2-83 3-4 3-80 4-5 4-6 6-7 7-8 7-9 8-11 9-10 9-71
10-11 10-68 11-24 12-13 12-16 12-23 13-14 13-76 14-15 14-79 15-16 15-17
17-18 18-19 18-20
19-22 20-21 20-72 21-22 21-75 22-24 25-26 25-29 25-47 26-27 26-67 27-28
27-64 28-29
28-30 30-31 31-32 31-33 32-35 33-34 33-55 34-35 34-52 35-48 36-37 36-40
36-47 37-38
37-60 38-39 38-63 39-40 39-41 41-42 42-43 42-44 43-46 44-45 44-56 45-46
45-59 46-48
52-53 53-54 54-55 56-57 57-58 58-59 60-61 61-62 62-63 64-65 65-66 66-67
68-69 69-70
70-71 72-73 73-74 74-75 76-77 77-78 78-79 80-81 81-82 82-83 86-87 86-91

```
87-88  88-89
89-90  90-91
exact/norm bonds :
1-2  1-5  1-23  2-3  2-83  3-4  3-80  4-5  4-6  6-7  7-8  7-9  8-11  9-10  9-71
10-11  10-68  11-24  12-13  12-16  12-23  13-14  13-76  14-15  14-79  15-16  15-17
16-51  17-18  18-19
18-20  19-22  20-21  20-72  21-22  21-75  22-24  25-26  25-29  25-47  26-27  26-67
27-28  27-64
28-29  28-30  30-31  31-32  31-33  32-35  33-34  33-55  34-35  34-52  35-48  36-37
36-40  36-47
37-38  37-60  38-39  38-63  39-40  39-41  41-42  42-43  42-44  43-46  43-49  44-45
44-56  45-46
45-59  46-48  49-50  50-51  52-53  53-54  54-55  56-57  57-58  58-59  60-61  61-62
62-63  64-65
65-66  66-67  68-69  69-70  70-71  72-73  73-74  74-75  76-77  77-78  78-79  80-81
81-82  82-83
84-85  90-92  94-95  94-96  97-98  97-99  105-106  105-107  108-109  108-110
normalized bonds :
86-87  86-91  87-88  88-89  89-90  90-91

G1:N,CN,NO2,X,Ak,[*1],[*2],[*3],[*4],[*5],[*6],[*7]

Match level :
1:Atom  2:Atom  3:Atom  4:Atom  5:Atom  6:Atom  7:Atom  8:Atom  9:Atom  10:Atom
11:Atom  12:Atom  13:Atom  14:Atom  15:Atom  16:Atom  17:Atom  18:Atom  19:Atom
20:Atom  21:Atom
22:Atom  23:Atom  24:Atom  25:Atom  26:Atom  27:Atom  28:Atom  29:Atom  30:Atom
31:Atom  32:Atom
33:Atom  34:Atom  35:Atom  36:Atom  37:Atom  38:Atom  39:Atom  40:Atom  41:Atom
42:Atom  43:Atom
44:Atom  45:Atom  46:Atom  47:Atom  48:Atom  49:CLASS  50:CLASS  51:CLASS  52:Atom
53:Atom  54:Atom
55:Atom  56:Atom  57:Atom  58:Atom  59:Atom  60:Atom  61:Atom  62:Atom  63:Atom
64:Atom  65:Atom
66:Atom  67:Atom  68:Atom  69:Atom  70:Atom  71:Atom  72:Atom  73:Atom  74:Atom
75:Atom  76:Atom
77:Atom  78:Atom  79:Atom  80:Atom  81:Atom  82:Atom  83:Atom  84:CLASS  85:CLASS
86:Atom  87:Atom
88:Atom  89:Atom  90:Atom  91:Atom  92:CLASS  93:Atom  94:CLASS  95:CLASS  96:CLASS
97:CLASS
98:CLASS  99:CLASS  105:CLASS  106:CLASS  107:CLASS  108:CLASS  109:CLASS
110:CLASS  115:CLASS  116:CLASS
118:CLASS  119:CLASS  120:CLASS  121:CLASS  122:CLASS  123:CLASS  125:Atom
126:Atom  127:Atom
128:Atom  129:Atom  130:Atom  131:Atom  132:Atom
Generic attributes :
93:
Saturation              : Unsaturated

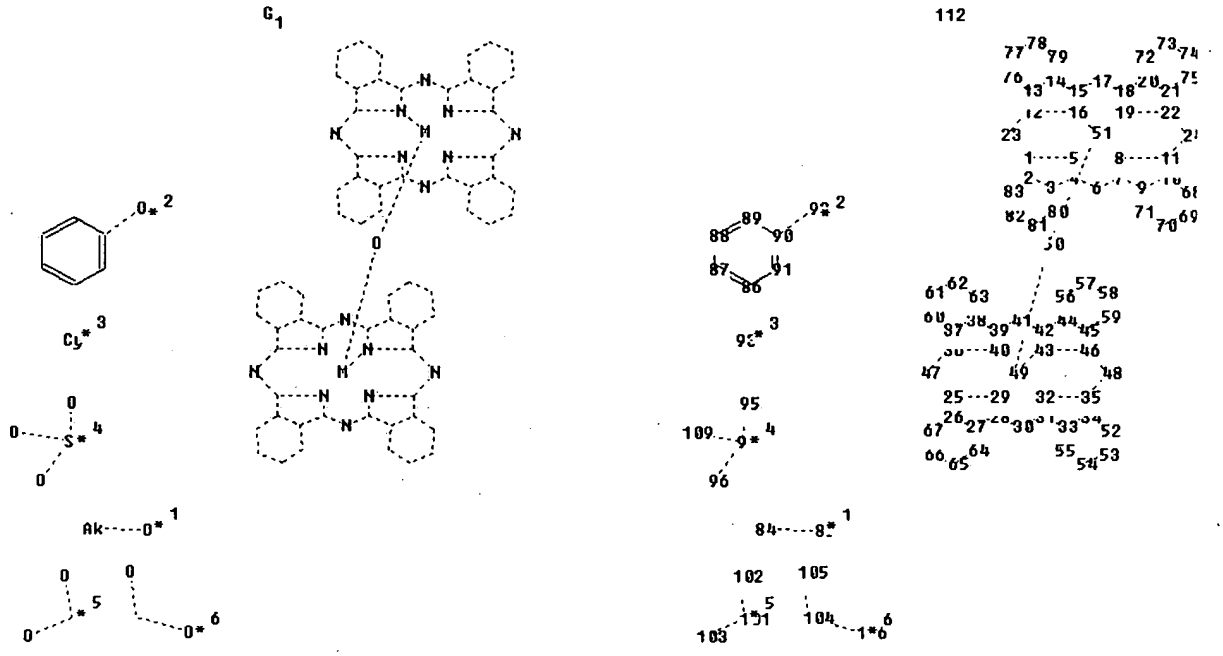


L17          58 SEA FILE=REGISTRY SUB=L5 SSS FUL L15
L32             STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY -  AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation:
```

Uploading L32b.str



chain nodes :
50 84 85 92 93 94 95 96 101 102 103 104 105 106 109 112
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23
24 25 26 27 28 29 30 31 32 33 34 35 36 37 38 39 40 41 42 43 44
45 46 47 48
52 53 54 55 56 57 58 59 60 61 62 63 64 65 66 67 68 69 70 71 72
73 74 75
76 77 78 79 80 81 82 83 86 87 88 89 90 91
ring/chain nodes :
49 51
chain bonds :
49-50 50-51 84-85 90-92 94-95 94-96 94-109 101-102 101-103 104-105 104-
106

ring/chain bonds :
16-51 43-49
ring bonds :
1-2 1-5 1-23 2-3 2-83 3-4 3-80 4-5 4-6 6-7 7-8 7-9 8-11 9-10 9-71
10-11 10-68 11-24 12-13 12-16 12-23 13-14 13-76 14-15 14-79 15-16 15-17
17-18 18-19 18-20
19-22 20-21 20-72 21-22 21-75 22-24 25-26 25-29 25-47 26-27 26-67 27-28
27-64 28-29
28-30 30-31 31-32 31-33 32-35 33-34 33-55 34-35 34-52 35-48 36-37 36-40
36-47 37-38
37-60 38-39 38-63 39-40 39-41 41-42 42-43 42-44 43-46 44-45 44-56 45-46
45-59 46-48
52-53 53-54 54-55 56-57 57-58 58-59 60-61 61-62 62-63 64-65 65-66 66-67
68-69 69-70
70-71 72-73 73-74 74-75 76-77 77-78 78-79 80-81 81-82 82-83 86-87 86-91

```
87-88  88-89
89-90  90-91
exact/norm bonds :
1-2  1-5  1-23  2-3  2-83  3-4  3-80  4-5  4-6  6-7  7-8  7-9  8-11  9-10  9-71
10-11  10-68  11-24  12-13  12-16  12-23  13-14  13-76  14-15  14-79  15-16  15-17
16-51  17-18  18-19
18-20  19-22  20-21  20-72  21-22  21-75  22-24  25-26  25-29  25-47  26-27  26-67
27-28  27-64
28-29  28-30  30-31  31-32  31-33  32-35  33-34  33-55  34-35  34-52  35-48  36-37
36-40  36-47
37-38  37-60  38-39  38-63  39-40  39-41  41-42  42-43  42-44  43-46  43-49  44-45
44-56  45-46
45-59  46-48  49-50  50-51  52-53  53-54  54-55  56-57  57-58  58-59  60-61  61-62
62-63  64-65
65-66  66-67  68-69  69-70  70-71  72-73  73-74  74-75  76-77  77-78  78-79  80-81
81-82  82-83
84-85  90-92  94-95  94-96  94-109  101-102  101-103  104-105  104-106
normalized bonds :
86-87  86-91  87-88  88-89  89-90  90-91


G1:X,Ak,CN,NO2,N,[*1],[*2],[*3],[*4],[*5],[*6]

Match level :
1:Atom  2:Atom  3:Atom  4:Atom  5:Atom  6:Atom  7:Atom  8:Atom  9:Atom  10:Atom
11:Atom  12:Atom  13:Atom  14:Atom  15:Atom  16:Atom  17:Atom  18:Atom  19:Atom
20:Atom  21:Atom
22:Atom  23:Atom  24:Atom  25:Atom  26:Atom  27:Atom  28:Atom  29:Atom  30:Atom
31:Atom  32:Atom
33:Atom  34:Atom  35:Atom  36:Atom  37:Atom  38:Atom  39:Atom  40:Atom  41:Atom
42:Atom  43:Atom
44:Atom  45:Atom  46:Atom  47:Atom  48:Atom  49:CLASS  50:CLASS  51:CLASS  52:Atom
53:Atom  54:Atom
55:Atom  56:Atom  57:Atom  58:Atom  59:Atom  60:Atom  61:Atom  62:Atom  63:Atom
64:Atom  65:Atom
66:Atom  67:Atom  68:Atom  69:Atom  70:Atom  71:Atom  72:Atom  73:Atom  74:Atom
75:Atom  76:Atom
77:Atom  78:Atom  79:Atom  80:Atom  81:Atom  82:Atom  83:Atom  84:CLASS  85:CLASS
86:Atom  87:Atom
88:Atom  89:Atom  90:Atom  91:Atom  92:CLASS  93:Atom  94:CLASS  95:CLASS  96:CLASS
101:CLASS
102:CLASS  103:CLASS  104:CLASS  105:CLASS  106:CLASS  109:CLASS  112:CLASS
Generic attributes :
93:
Saturation              : Unsaturated

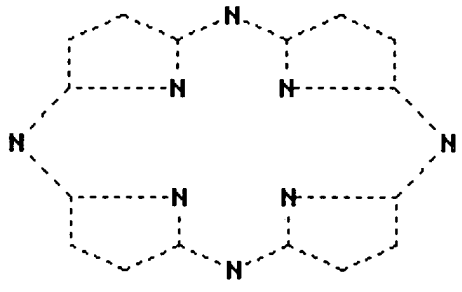


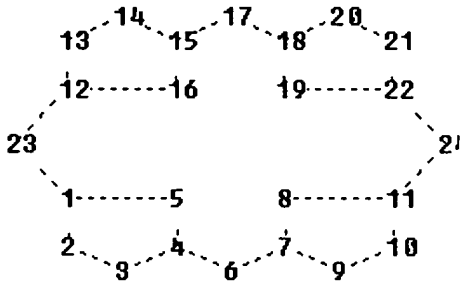

L34          154 SEA FILE=REGISTRY SUB=L5 SSS FUL L32
L40            1 SEA FILE=REGISTRY ABB=ON  PLU=ON  L17 AND HYDROXIDE/CNS
L41            6 SEA FILE=REGISTRY ABB=ON  PLU=ON  L34 AND HYDROXIDE/CNS
L42            1 SEA FILE=REGISTRY ABB=ON  PLU=ON  L34 AND SULFATE/CNS
L46            7 SEA FILE=REGISTRY ABB=ON  PLU=ON  (L40 OR L41 OR L42)
L50            5 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  L46

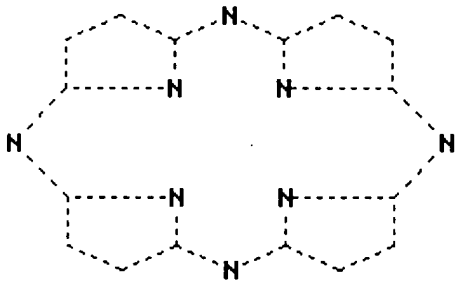

=> d stat que L67
L4              STR
```

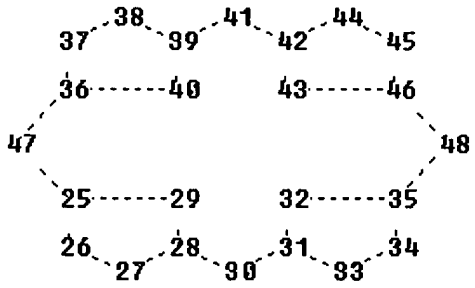
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation:
Uploading L4b.str









ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23
24 25 26 27 28 29 30 31 32 33 34 35 36 37 38 39 40 41 42 43 44
45 46 47 48

ring bonds :
1-2 1-5 1-23 2-3 3-4 4-5 4-6 6-7 7-8 7-9 8-11 9-10 10-11 11-24 12-13
12-16 12-23 13-14 14-15 15-16 15-17 17-18 18-19 18-20 19-22 20-21 21-22
22-24 25-26
25-29 25-47 26-27 27-28 28-29 28-30 30-31 31-32 31-33 32-35 33-34 34-35
35-48 36-37
36-40 36-47 37-38 38-39 39-40 39-41 41-42 42-43 42-44 43-46 44-45 45-46
46-48
exact/norm bonds :
1-2 1-5 1-23 2-3 3-4 4-5 4-6 6-7 7-8 7-9 8-11 9-10 10-11 11-24 12-13
12-16 12-23 13-14 14-15 15-16 15-17 17-18 18-19 18-20 19-22 20-21 21-22
22-24 25-26
25-29 25-47 26-27 27-28 28-29 28-30 30-31 31-32 31-33 32-35 33-34 34-35
35-48 36-37
36-40 36-47 37-38 38-39 39-40 39-41 41-42 42-43 42-44 43-46 44-45 45-46
46-48

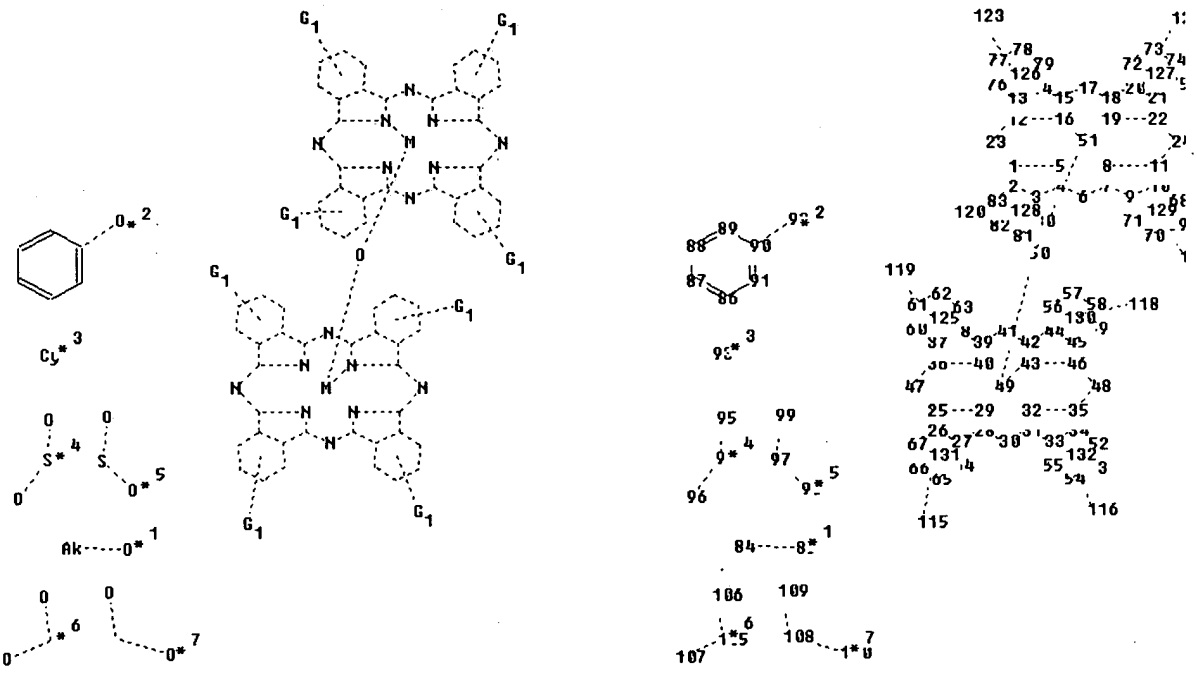
Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom

11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom
20:Atom 21:Atom
22:Atom 23:Atom 24:Atom 25:Atom 26:Atom 27:Atom 28:Atom 29:Atom 30:Atom
31:Atom 32:Atom
33:Atom 34:Atom 35:Atom 36:Atom 37:Atom 38:Atom 39:Atom 40:Atom 41:Atom
42:Atom 43:Atom
44:Atom 45:Atom 46:Atom 47:Atom 48:Atom

L5 2661 SEA FILE=REGISTRY SSS FUL L4
L15 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation:
Uploading L15b.str



chain nodes :
50 84 85 92 93 94 95 96 97 98 99 105 106 107 108 109 110 115 116
118 119 120 121 122 123
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23
24 25 26 27 28 29 30 31 32 33 34 35 36 37 38 39 40 41 42 43 44
45 46 47 48
52 53 54 55 56 57 58 59 60 61 62 63 64 65 66 67 68 69 70 71 72
73 74 75
76 77 78 79 80 81 82 83 86 87 88 89 90 91
ring/chain nodes :
49 51

chain bonds :
49-50 50-51 84-85 90-92 94-95 94-96 97-98 97-99 105-106 105-107 108-109
108-110
ring/chain bonds :
16-51 43-49
ring bonds :
1-2 1-5 1-23 2-3 2-83 3-4 3-80 4-5 4-6 6-7 7-8 7-9 8-11 9-10 9-71
10-11 10-68 11-24 12-13 12-16 12-23 13-14 13-76 14-15 14-79 15-16 15-17
17-18 18-19 18-20
19-22 20-21 20-72 21-22 21-75 22-24 25-26 25-29 25-47 26-27 26-67 27-28
27-64 28-29
28-30 30-31 31-32 31-33 32-35 33-34 33-55 34-35 34-52 35-48 36-37 36-40
36-47 37-38
37-60 38-39 38-63 39-40 39-41 41-42 42-43 42-44 43-46 44-45 44-56 45-46
45-59 46-48
52-53 53-54 54-55 56-57 57-58 58-59 60-61 61-62 62-63 64-65 65-66 66-67
68-69 69-70
70-71 72-73 73-74 74-75 76-77 77-78 78-79 80-81 81-82 82-83 86-87 86-91
87-88 88-89
89-90 90-91
exact/norm bonds :
1-2 1-5 1-23 2-3 2-83 3-4 3-80 4-5 4-6 6-7 7-8 7-9 8-11 9-10 9-71
10-11 10-68 11-24 12-13 12-16 12-23 13-14 13-76 14-15 14-79 15-16 15-17
16-51 17-18 18-19
18-20 19-22 20-21 20-72 21-22 21-75 22-24 25-26 25-29 25-47 26-27 26-67
27-28 27-64
28-29 28-30 30-31 31-32 31-33 32-35 33-34 33-55 34-35 34-52 35-48 36-37
36-40 36-47
37-38 37-60 38-39 38-63 39-40 39-41 41-42 42-43 42-44 43-46 43-49 44-45
44-56 45-46
45-59 46-48 49-50 50-51 52-53 53-54 54-55 56-57 57-58 58-59 60-61 61-62
62-63 64-65
65-66 66-67 68-69 69-70 70-71 72-73 73-74 74-75 76-77 77-78 78-79 80-81
81-82 82-83
84-85 90-92 94-95 94-96 97-98 97-99 105-106 105-107 108-109 108-110
normalized bonds :
86-87 86-91 87-88 88-89 89-90 90-91

G1:N,CN,NO2,X,Ak,[*1],[*2],[*3],[*4],[*5],[*6],[*7]

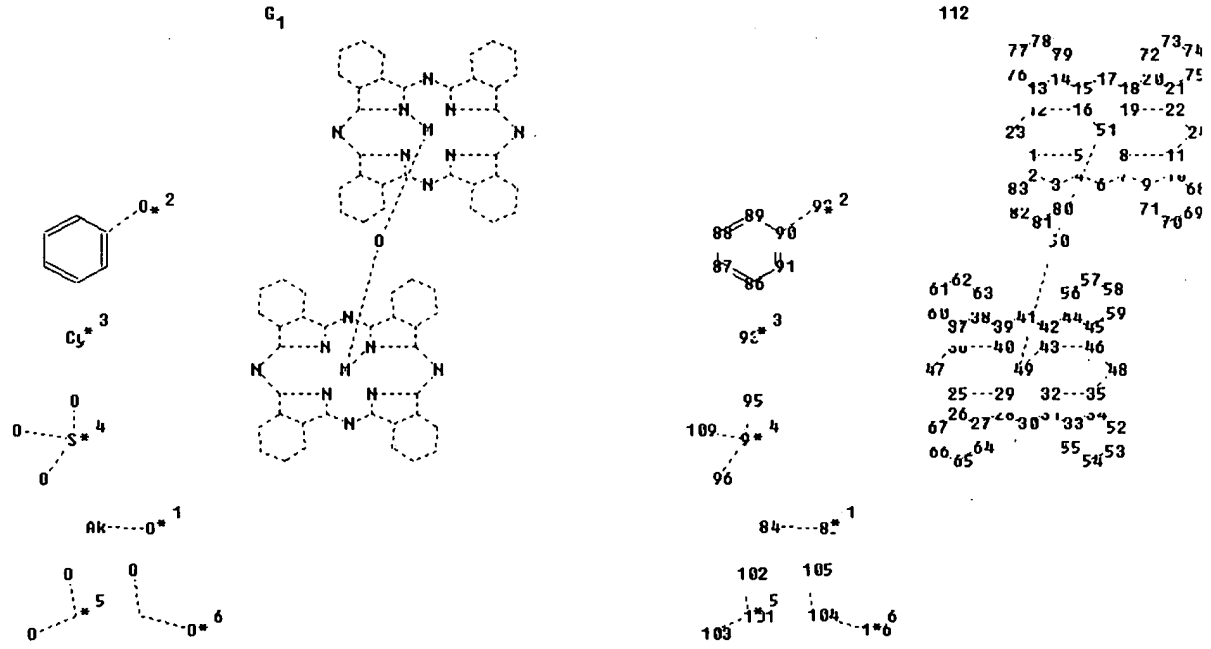
Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom
20:Atom 21:Atom
22:Atom 23:Atom 24:Atom 25:Atom 26:Atom 27:Atom 28:Atom 29:Atom 30:Atom
31:Atom 32:Atom
33:Atom 34:Atom 35:Atom 36:Atom 37:Atom 38:Atom 39:Atom 40:Atom 41:Atom
42:Atom 43:Atom
44:Atom 45:Atom 46:Atom 47:Atom 48:Atom 49:CLASS 50:CLASS 51:CLASS 52:Atom
53:Atom 54:Atom
55:Atom 56:Atom 57:Atom 58:Atom 59:Atom 60:Atom 61:Atom 62:Atom 63:Atom
64:Atom 65:Atom
66:Atom 67:Atom 68:Atom 69:Atom 70:Atom 71:Atom 72:Atom 73:Atom 74:Atom
75:Atom 76:Atom
77:Atom 78:Atom 79:Atom 80:Atom 81:Atom 82:Atom 83:Atom 84:CLASS 85:CLASS
86:Atom 87:Atom
88:Atom 89:Atom 90:Atom 91:Atom 92:CLASS 93:Atom 94:CLASS 95:CLASS 96:CLASS
97:CLASS
98:CLASS 99:CLASS 105:CLASS 106:CLASS 107:CLASS 108:CLASS 109:CLASS

110:CLASS 115:CLASS 116:CLASS
118:CLASS 119:CLASS 120:CLASS 121:CLASS 122:CLASS 123:CLASS 125:Atom
126:Atom 127:Atom
128:Atom 129:Atom 130:Atom 131:Atom 132:Atom
Generic attributes :
93:
Saturation : Unsaturated

L17 58 SEA FILE=REGISTRY SUB=L5 SSS FUL L15
L32 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation:
Uploading L32b.str



chain nodes :
50 84 85 92 93 94 95 96 101 102 103 104 105 106 109 112
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23
24 25 26 27 28 29 30 31 32 33 34 35 36 37 38 39 40 41 42 43 44
45 46 47 48
52 53 54 55 56 57 58 59 60 61 62 63 64 65 66 67 68 69 70 71 72
73 74 75
76 77 78 79 80 81 82 83 86 87 88 89 90 91
ring/chain nodes :
49 51
chain bonds :

49-50 50-51 84-85 90-92 94-95 94-96 94-109 101-102 101-103 104-105 104-106

ring/chain bonds :
16-51 43-49
ring bonds :
1-2 1-5 1-23 2-3 2-83 3-4 3-80 4-5 4-6 6-7 7-8 7-9 8-11 9-10 9-71
10-11 10-68 11-24 12-13 12-16 12-23 13-14 13-76 14-15 14-79 15-16 15-17
17-18 18-19 18-20
19-22 20-21 20-72 21-22 21-75 22-24 25-26 25-29 25-47 26-27 26-67 27-28
27-64 28-29
28-30 30-31 31-32 31-33 32-35 33-34 33-55 34-35 34-52 35-48 36-37 36-40
36-47 37-38
37-60 38-39 38-63 39-40 39-41 41-42 42-43 42-44 43-46 44-45 44-56 45-46
45-59 46-48
52-53 53-54 54-55 56-57 57-58 58-59 60-61 61-62 62-63 64-65 65-66 66-67
68-69 69-70
70-71 72-73 73-74 74-75 76-77 77-78 78-79 80-81 81-82 82-83 86-87 86-91
87-88 88-89
89-90 90-91
exact/norm bonds :
1-2 1-5 1-23 2-3 2-83 3-4 3-80 4-5 4-6 6-7 7-8 7-9 8-11 9-10 9-71
10-11 10-68 11-24 12-13 12-16 12-23 13-14 13-76 14-15 14-79 15-16 15-17
16-51 17-18 18-19
18-20 19-22 20-21 20-72 21-22 21-75 22-24 25-26 25-29 25-47 26-27 26-67
27-28 27-64
28-29 28-30 30-31 31-32 31-33 32-35 33-34 33-55 34-35 34-52 35-48 36-37
36-40 36-47
37-38 37-60 38-39 38-63 39-40 39-41 41-42 42-43 42-44 43-46 43-49 44-45
44-56 45-46
45-59 46-48 49-50 50-51 52-53 53-54 54-55 56-57 57-58 58-59 60-61 61-62
62-63 64-65
65-66 66-67 68-69 69-70 70-71 72-73 73-74 74-75 76-77 77-78 78-79 80-81
81-82 82-83
84-85 90-92 94-95 94-96 94-109 101-102 101-103 104-105 104-106
normalized bonds :
86-87 86-91 87-88 88-89 89-90 90-91

G1:X,Ak,CN,NO2,N,[*1],[*2],[*3],[*4],[*5],[*6]

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom
20:Atom 21:Atom
22:Atom 23:Atom 24:Atom 25:Atom 26:Atom 27:Atom 28:Atom 29:Atom 30:Atom
31:Atom 32:Atom
33:Atom 34:Atom 35:Atom 36:Atom 37:Atom 38:Atom 39:Atom 40:Atom 41:Atom
42:Atom 43:Atom
44:Atom 45:Atom 46:Atom 47:Atom 48:Atom 49:CLASS 50:CLASS 51:CLASS 52:Atom
53:Atom 54:Atom
55:Atom 56:Atom 57:Atom 58:Atom 59:Atom 60:Atom 61:Atom 62:Atom 63:Atom
64:Atom 65:Atom
66:Atom 67:Atom 68:Atom 69:Atom 70:Atom 71:Atom 72:Atom 73:Atom 74:Atom
75:Atom 76:Atom
77:Atom 78:Atom 79:Atom 80:Atom 81:Atom 82:Atom 83:Atom 84:CLASS 85:CLASS
86:Atom 87:Atom
88:Atom 89:Atom 90:Atom 91:Atom 92:CLASS 93:Atom 94:CLASS 95:CLASS 96:CLASS
101:CLASS
102:CLASS 103:CLASS 104:CLASS 105:CLASS 106:CLASS 109:CLASS 112:CLASS

```
Generic attributes :
93:
Saturation              : Unsaturated

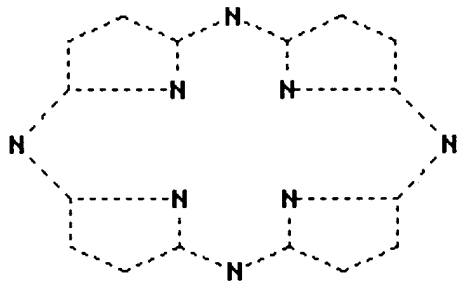


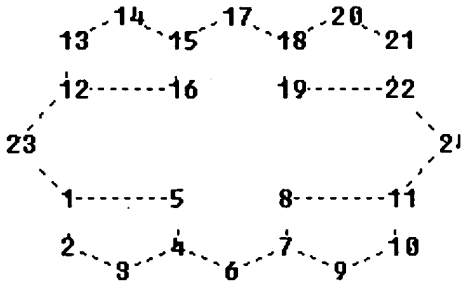
L34          154 SEA FILE=REGISTRY SUB=L5 SSS FUL L32
L40            1 SEA FILE=REGISTRY ABB=ON  PLU=ON  L17 AND HYDROXIDE/CNS
L41            6 SEA FILE=REGISTRY ABB=ON  PLU=ON  L34 AND HYDROXIDE/CNS
L42            1 SEA FILE=REGISTRY ABB=ON  PLU=ON  L34 AND SULFATE/CNS
L44          154 SEA FILE=REGISTRY ABB=ON  PLU=ON  L17 OR L34
L46            7 SEA FILE=REGISTRY ABB=ON  PLU=ON  (L40 OR L41 OR L42)
L50            5 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  L46
L57            1 SEA FILE=REGISTRY ABB=ON  PLU=ON  HYDROXIDE/CN
L58            1 SEA FILE=REGISTRY ABB=ON  PLU=ON  SULFATE/CN
L59            1 SEA FILE=REGISTRY ABB=ON  PLU=ON  CHLORIDE/CN
L60            0 SEA FILE=REGISTRY ABB=ON  PLU=ON  H S O/ELF
L61        30961 SEA FILE=REGISTRY ABB=ON  PLU=ON  H O S/ELF
L62        30964 SEA FILE=REGISTRY ABB=ON  PLU=ON  (L57 OR L58 OR L59 OR L60 OR
                 L61)
L63           83 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  L44
L64           50 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  L17
L65            4 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  L62 AND (L63 OR L64)
L66            4 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  L65 NOT L50
L67            1 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  L66 AND SULFATE/OBI

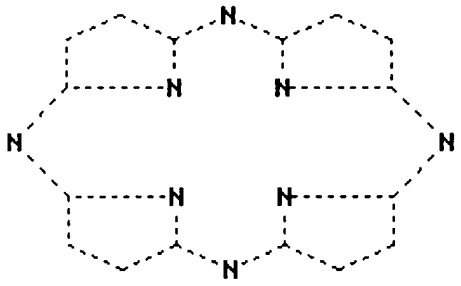

=> d stat que L69
L4               STR

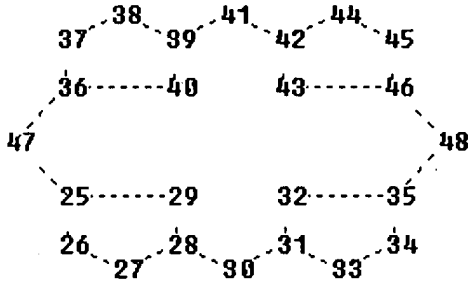
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY -  AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation:
Uploading L4b.str
```









ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23
24 25 26 27 28 29 30 31 32 33 34 35 36 37 38 39 40 41 42 43 44
45 46 47 48

ring bonds :
1-2 1-5 1-23 2-3 3-4 4-5 4-6 6-7 7-8 7-9 8-11 9-10 10-11 11-24 12-13
12-16 12-23 13-14 14-15 15-16 15-17 17-18 18-19 18-20 19-22 20-21 21-22
22-24 25-26
25-29 25-47 26-27 27-28 28-29 28-30 30-31 31-32 31-33 32-35 33-34 34-35
35-48 36-37
36-40 36-47 37-38 38-39 39-40 39-41 41-42 42-43 42-44 43-46 44-45 45-46
46-48
exact/norm bonds :
1-2 1-5 1-23 2-3 3-4 4-5 4-6 6-7 7-8 7-9 8-11 9-10 10-11 11-24 12-13
12-16 12-23 13-14 14-15 15-16 15-17 17-18 18-19 18-20 19-22 20-21 21-22
22-24 25-26
25-29 25-47 26-27 27-28 28-29 28-30 30-31 31-32 31-33 32-35 33-34 34-35
35-48 36-37
36-40 36-47 37-38 38-39 39-40 39-41 41-42 42-43 42-44 43-46 44-45 45-46
46-48

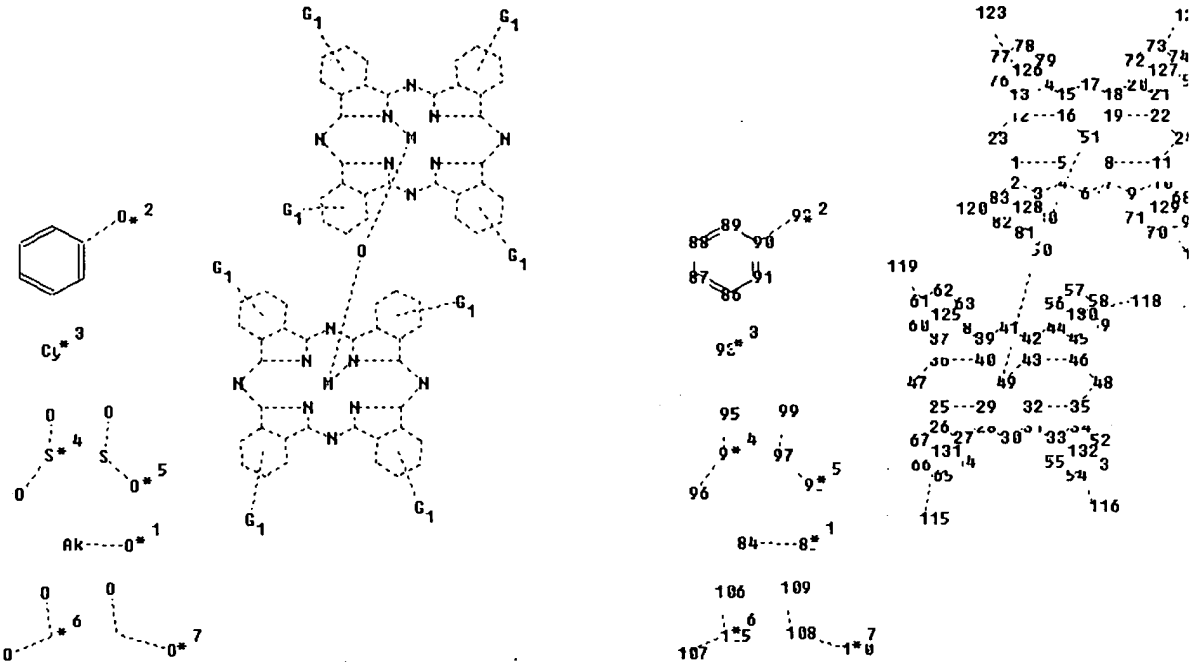
Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom
20:Atom 21:Atom
22:Atom 23:Atom 24:Atom 25:Atom 26:Atom 27:Atom 28:Atom 29:Atom 30:Atom
31:Atom 32:Atom
33:Atom 34:Atom 35:Atom 36:Atom 37:Atom 38:Atom 39:Atom 40:Atom 41:Atom

42:Atom 43:Atom
44:Atom 45:Atom 46:Atom 47:Atom 48:Atom

L5 2661 SEA FILE=REGISTRY SSS FUL L4
L15 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation:
Uploading L15b.str



chain nodes :
50 84 85 92 93 94 95 96 97 98 99 105 106 107 108 109 110 115 116
118 119 120 121 122 123
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23
24 25 26 27 28 29 30 31 32 33 34 35 36 37 38 39 40 41 42 43 44
45 46 47 48
52 53 54 55 56 57 58 59 60 61 62 63 64 65 66 67 68 69 70 71 72
73 74 75
76 77 78 79 80 81 82 83 86 87 88 89 90 91
ring/chain nodes :
49 51
chain bonds :
49-50 50-51 84-85 90-92 94-95 94-96 97-98 97-99 105-106 105-107 108-109
108-110
ring/chain bonds :
16-51 43-49

ring bonds :
1-2 1-5 1-23 2-3 2-83 3-4 3-80 4-5 4-6 6-7 7-8 7-9 8-11 9-10 9-71
10-11 10-68 11-24 12-13 12-16 12-23 13-14 13-76 14-15 14-79 15-16 15-17
17-18 18-19 18-20
19-22 20-21 20-72 21-22 21-75 22-24 25-26 25-29 25-47 26-27 26-67 27-28
27-64 28-29
28-30 30-31 31-32 31-33 32-35 33-34 33-55 34-35 34-52 35-48 36-37 36-40
36-47 37-38
37-60 38-39 38-63 39-40 39-41 41-42 42-43 42-44 43-46 44-45 44-56 45-46
45-59 46-48
52-53 53-54 54-55 56-57 57-58 58-59 60-61 61-62 62-63 64-65 65-66 66-67
68-69 69-70
70-71 72-73 73-74 74-75 76-77 77-78 78-79 80-81 81-82 82-83 86-87 86-91
87-88 88-89
89-90 90-91
exact/norm bonds :
1-2 1-5 1-23 2-3 2-83 3-4 3-80 4-5 4-6 6-7 7-8 7-9 8-11 9-10 9-71
10-11 10-68 11-24 12-13 12-16 12-23 13-14 13-76 14-15 14-79 15-16 15-17
16-51 17-18 18-19
18-20 19-22 20-21 20-72 21-22 21-75 22-24 25-26 25-29 25-47 26-27 26-67
27-28 27-64
28-29 28-30 30-31 31-32 31-33 32-35 33-34 33-55 34-35 34-52 35-48 36-37
36-40 36-47
37-38 37-60 38-39 38-63 39-40 39-41 41-42 42-43 42-44 43-46 43-49 44-45
44-56 45-46
45-59 46-48 49-50 50-51 52-53 53-54 54-55 56-57 57-58 58-59 60-61 61-62
62-63 64-65
65-66 66-67 68-69 69-70 70-71 72-73 73-74 74-75 76-77 77-78 78-79 80-81
81-82 82-83
84-85 90-92 94-95 94-96 97-98 97-99 105-106 105-107 108-109 108-110
normalized bonds :
86-87 86-91 87-88 88-89 89-90 90-91

G1:N,CN,NO2,X,Ak,[*1],[*2],[*3],[*4],[*5],[*6],[*7]

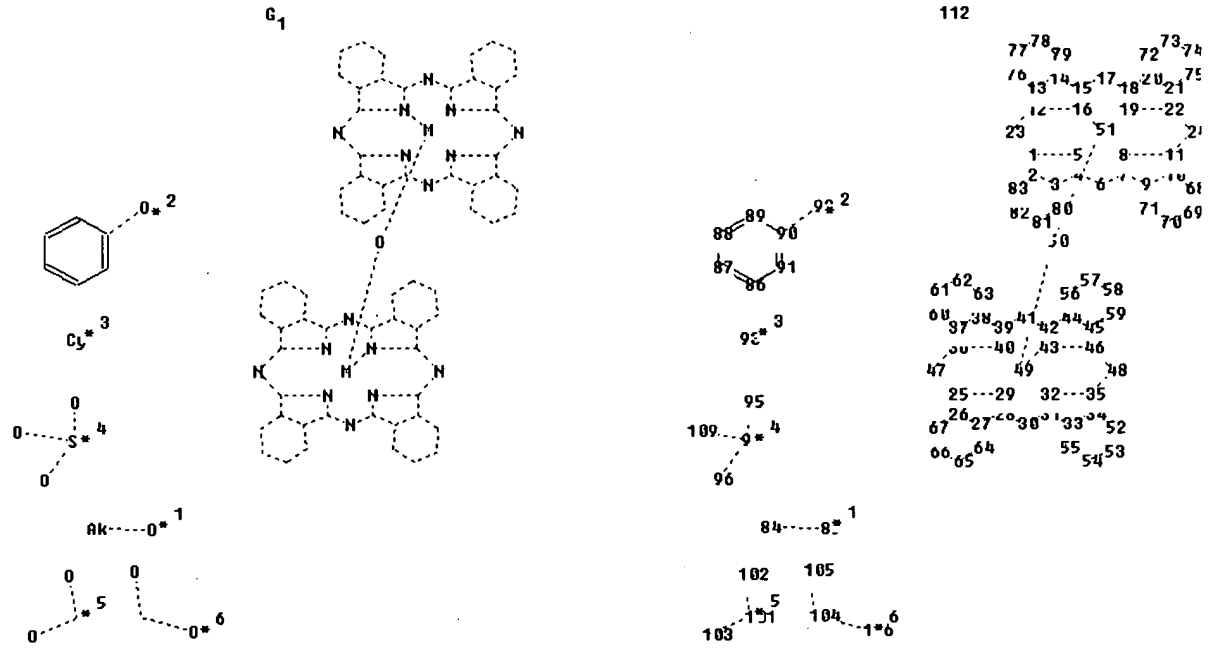
Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom
20:Atom 21:Atom
22:Atom 23:Atom 24:Atom 25:Atom 26:Atom 27:Atom 28:Atom 29:Atom 30:Atom
31:Atom 32:Atom
33:Atom 34:Atom 35:Atom 36:Atom 37:Atom 38:Atom 39:Atom 40:Atom 41:Atom
42:Atom 43:Atom
44:Atom 45:Atom 46:Atom 47:Atom 48:Atom 49:CLASS 50:CLASS 51:CLASS 52:Atom
53:Atom 54:Atom
55:Atom 56:Atom 57:Atom 58:Atom 59:Atom 60:Atom 61:Atom 62:Atom 63:Atom
64:Atom 65:Atom
66:Atom 67:Atom 68:Atom 69:Atom 70:Atom 71:Atom 72:Atom 73:Atom 74:Atom
75:Atom 76:Atom
77:Atom 78:Atom 79:Atom 80:Atom 81:Atom 82:Atom 83:Atom 84:CLASS 85:CLASS
86:Atom 87:Atom
88:Atom 89:Atom 90:Atom 91:Atom 92:CLASS 93:Atom 94:CLASS 95:CLASS 96:CLASS
97:CLASS
98:CLASS 99:CLASS 105:CLASS 106:CLASS 107:CLASS 108:CLASS 109:CLASS
110:CLASS 115:CLASS 116:CLASS
118:CLASS 119:CLASS 120:CLASS 121:CLASS 122:CLASS 123:CLASS 125:Atom
126:Atom 127:Atom
128:Atom 129:Atom 130:Atom 131:Atom 132:Atom
Generic attributes :

93:
Saturation : Unsaturated

L17 58 SEA FILE=REGISTRY SUB=L5 SSS FUL L15
L32 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation:
Uploading L32b.str



chain nodes :
50 84 85 92 93 94 95 96 101 102 103 104 105 106 109 112
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23
24 25 26 27 28 29 30 31 32 33 34 35 36 37 38 39 40 41 42 43 44
45 46 47 48
52 53 54 55 56 57 58 59 60 61 62 63 64 65 66 67 68 69 70 71 72
73 74 75
76 77 78 79 80 81 82 83 86 87 88 89 90 91
ring/chain nodes :
49 51
chain bonds :
49-50 50-51 84-85 90-92 94-95 94-96 94-109 101-102 101-103 104-105 104-
106

ring/chain bonds :
16-51 43-49

ring bonds :
1-2 1-5 1-23 2-3 2-83 3-4 3-80 4-5 4-6 6-7 7-8 7-9 8-11 9-10 9-71
10-11 10-68 11-24 12-13 12-16 12-23 13-14 13-76 14-15 14-79 15-16 15-17
17-18 18-19 18-20
19-22 20-21 20-72 21-22 21-75 22-24 25-26 25-29 25-47 26-27 26-67 27-28
27-64 28-29
28-30 30-31 31-32 31-33 32-35 33-34 33-55 34-35 34-52 35-48 36-37 36-40
36-47 37-38
37-60 38-39 38-63 39-40 39-41 41-42 42-43 42-44 43-46 44-45 44-56 45-46
45-59 46-48
52-53 53-54 54-55 56-57 57-58 58-59 60-61 61-62 62-63 64-65 65-66 66-67
68-69 69-70
70-71 72-73 73-74 74-75 76-77 77-78 78-79 80-81 81-82 82-83 86-87 86-91
87-88 88-89
89-90 90-91
exact/norm bonds :
1-2 1-5 1-23 2-3 2-83 3-4 3-80 4-5 4-6 6-7 7-8 7-9 8-11 9-10 9-71
10-11 10-68 11-24 12-13 12-16 12-23 13-14 13-76 14-15 14-79 15-16 15-17
16-51 17-18 18-19
18-20 19-22 20-21 20-72 21-22 21-75 22-24 25-26 25-29 25-47 26-27 26-67
27-28 27-64
28-29 28-30 30-31 31-32 31-33 32-35 33-34 33-55 34-35 34-52 35-48 36-37
36-40 36-47
37-38 37-60 38-39 38-63 39-40 39-41 41-42 42-43 42-44 43-46 43-49 44-45
44-56 45-46
45-59 46-48 49-50 50-51 52-53 53-54 54-55 56-57 57-58 58-59 60-61 61-62
62-63 64-65
65-66 66-67 68-69 69-70 70-71 72-73 73-74 74-75 76-77 77-78 78-79 80-81
81-82 82-83
84-85 90-92 94-95 94-96 94-109 101-102 101-103 104-105 104-106
normalized bonds :
86-87 86-91 87-88 88-89 89-90 90-91

G1:X,Ak,CN,NO2,N,[*1],[*2],[*3],[*4],[*5],[*6]

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom
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22:Atom 23:Atom 24:Atom 25:Atom 26:Atom 27:Atom 28:Atom 29:Atom 30:Atom
31:Atom 32:Atom
33:Atom 34:Atom 35:Atom 36:Atom 37:Atom 38:Atom 39:Atom 40:Atom 41:Atom
42:Atom 43:Atom
44:Atom 45:Atom 46:Atom 47:Atom 48:Atom 49:CLASS 50:CLASS 51:CLASS 52:Atom
53:Atom 54:Atom
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64:Atom 65:Atom
66:Atom 67:Atom 68:Atom 69:Atom 70:Atom 71:Atom 72:Atom 73:Atom 74:Atom
75:Atom 76:Atom
77:Atom 78:Atom 79:Atom 80:Atom 81:Atom 82:Atom 83:Atom 84:CLASS 85:CLASS
86:Atom 87:Atom
88:Atom 89:Atom 90:Atom 91:Atom 92:CLASS 93:Atom 94:CLASS 95:CLASS 96:CLASS
101:CLASS
102:CLASS 103:CLASS 104:CLASS 105:CLASS 106:CLASS 109:CLASS 112:CLASS
Generic attributes :
93:
Saturation : Unsaturated

```
L34          154 SEA FILE=REGISTRY SUB=L5 SSS FUL L32
L44          154 SEA FILE=REGISTRY ABB=ON  PLU=ON  L17 OR L34
L63           83 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  L44
L64           50 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  L17
L68       581403 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  CHARGE/BI
L69            8 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  (L63 OR L64) AND L68


=> s (L38 or L50 or L67 or L69) not (L72 or L73)
L75          9 (L38 OR L50 OR L67 OR L69) NOT (L72 OR L73)

=> d ibib abs hitind hitstr L75 1-9

L75  ANSWER 1 OF 9  ZCAPLUS  COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER:         2005:981679  ZCAPLUS  Full-text
DOCUMENT NUMBER:          143:485704
TITLE:                    Photoredox reaction of (Pcts)FeIII(O22-)FeIII( Pcts)
                          with PctsH2 = phthalocyaninetetrasulfonate induced by
                          peroxide to Fe(III) charge transfer
                          excitation
AUTHOR(S):                Kunkely, Horst; Vogler, Arnd
CORPORATE SOURCE:         Institut fuer Anorganische Chemie, Universitaet
                          Regensburg, Regensburg, D-93040, Germany
SOURCE:                   Inorganica Chimica Acta (2005), 358(13), 4086-4088
                          CODEN: ICHAA3; ISSN: 0020-1693
PUBLISHER:                Elsevier B.V.
DOCUMENT TYPE:            Journal
LANGUAGE:                 English
AB    The binuclear complex (Pcts)FeIII(O22-)FeIII( Pcts ) where PctsH =
      phthalocyaninetetrasulfonate is stable in aqueous solution for some time
      (.apprx.1 h) before it is irreversibly converted to (Pcts)FeIII-O-
      FeIII(Pcts). The photolysis of the peroxo complex in argon-saturated water
      leads to the release of oxygen and the formation of FeII(Pcts) with .vphi. = 5
      + 10-4 at λirr = 333 nm. It is suggested that this photoredox reaction
      originates from a peroxide to FeIII LMCT state. It is populated from Pcts IL
      states which are initially reached by light absorption.
CC    74-1 (Radiation Chemistry, Photochemistry, and Photographic and Other
      Reprographic Processes)
IT    Charge transfer transition
         (ligand-to-metal; photolysis of binuclear iron
         phthalocyaninetetrasulfonate peroxo complex in argon-saturated aqueous
solution)
IT    7782-44-7P, Oxygen, properties 721882-48-0P
      RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
         (photoproduct; photolysis of binuclear iron
         phthalocyaninetetrasulfonate peroxo complex in argon-saturated aqueous
solution)
IT    721882-48-0P
      RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
         (photoproduct; photolysis of binuclear iron
         phthalocyaninetetrasulfonate peroxo complex in argon-saturated aqueous
solution)
RN    721882-48-0  ZCAPLUS
CN    Ferrate(8-), μ-oxobis[29H,31H-phthalocyanine-2,9,16,23-tetrasulfonato(6-
      )-κN29,κN30,κN31,κN32]di- (9CI)  (CA INDEX NAME)
```

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
REFERENCE COUNT: 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L75 ANSWER 2 OF 9 ZCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1998:392995 ZCAPLUS Full-text
DOCUMENT NUMBER: 129:141830
TITLE: Anodic oxidation of cysteine catalyzed by nickel tetrasulfonated phthalocyanine immobilized on silica gel modified with titanium(IV) oxide
AUTHOR(S): Perez, Elizabeth F.; Kubota, Lauro T.; Tanaka, Auro A.; De Oliveira Neto, Graciliano
CORPORATE SOURCE: Instituto de Quimica, UNICAMP, Campinas, 13083-970, Brazil
SOURCE: Electrochimica Acta (1998), 43(12-13), 1665-1673
CODEN: ELCAAV; ISSN: 0013-4686
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB A chemical modified electrode constructed by mixing nickel tetrasulfonated phthalocyanine (NiTsPc) immobilized on modified silica gel with carbon paste showed a redox process with a midpoint potential of 0.44 V vs. SCE. Expts. carried out with different supporting electrolytes suggested an effect due to the nature of the anion. The solution pH does not affect the midpoint potential but the peak current increases when the pH is decreased. The immobilization procedure causes an increase in the monomeric form of the complex. The electrochem. property of NiTsPc adsorbed onto modified silica showed good stability even in acidic media (pH = 2) and the ability to catalyze the electrooxidn. of cysteine at 0.5 V vs. SCE.

CC 72-2 (Electrochemistry)
Section cross-reference(s): 22, 66, 67, 78

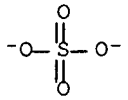
IT ***210690-34-9*** 210690-35-0
RL: FMU (Formation, unclassified); PRP (Properties); FORM (Formation, nonpreparative)
(effect of nitrogen or oxygen or air on Ni tetrasulfonated phthalocyanine dimer formation in aqueous solution: electrooxidn. of cysteine
catalyzed by Ni tetrasulfonated phthalocyanine immobilized on silica gel modified with Ti(IV) oxide)

IT 71-50-1, Acetic acid, ion(1-), uses 14127-61-8, Calcium(2+), uses 14797-55-8, Nitrate, uses 14797-73-0, Perchlorate 14798-03-9, Ammonium, uses ***14808-79-8***, ***Sulfate***, uses ***16887-00-6***, Chloride, uses 17341-24-1, Lithium(1+), uses 17341-25-2, Sodium(1+), uses 24203-36-9, Potassium(1+), uses
RL: NUU (Other use, unclassified); PRP (Properties); USES (Uses)
(midpoint potential for nickel tetrasulfonated phthalocyanine immobilized on silica gel modified with titanium(IV) oxide in solution containing)

IT ***210690-34-9***
RL: FMU (Formation, unclassified); PRP (Properties); FORM (Formation, nonpreparative)
(effect of nitrogen or oxygen or air on Ni tetrasulfonated phthalocyanine dimer formation in aqueous solution: electrooxidn. of cysteine
catalyzed by Ni tetrasulfonated phthalocyanine immobilized on silica gel modified with Ti(IV) oxide)

RN 210690-34-9 ZCAPLUS
CN Nickelate(10-), μ-oxobis[29H,31H-phthalocyanine-2,9,16,23-tetrasulfonato(6-)-κN29,κN30,κN31,κN32]di- (9CI)
(CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
IT *14808-79-8, Sulfate*, uses *16887-00-6*,
Chloride, uses
RL: NUU (Other use, unclassified); PRP (Properties); USES (Uses)
(midpoint potential for nickel tetrasulfonated phthalocyanine immobilized on silica gel modified with titanium(IV) oxide in solution containing)
RN 14808-79-8 ZCAPLUS
CN Sulfate (7CI, 8CI, 9CI) (CA INDEX NAME)



RN 16887-00-6 ZCAPLUS
CN Chloride (CA INDEX NAME)

Cl-

REFERENCE COUNT: 37 THERE ARE 37 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L75 ANSWER 3 OF 9 ZCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1996:81051 ZCAPLUS Full-text
DOCUMENT NUMBER: 124:218437
TITLE: Interaction of manganese phthalocyanine with tetracyanoquinodimethane in solution
AUTHOR(S): Sidorov, A. N.
CORPORATE SOURCE: Vavilov State Optical Inst., All-Russia Scientific Center, St. Petersburg, 193171, Russia
SOURCE: Russian Journal of Coordination Chemistry (Translation of Koordinatsionnaya Khimiya) (1995), 21(12), 898-900
CODEN: RJCCEY; ISSN: 1070-3284
PUBLISHER: MAIK Nauka/Interperiodica
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The interaction between the Mn(II) phthalocyanine complex (MnPc) and tetracyanoquinodimethane (TCNQ) in a solution of a THF-Et2O mixture was studied by electronic absorption spectroscopy. The interaction has the donor-acceptor nature, with the Mn atom as a donor. It is assumed that the reaction product has the MnIIIPc(TCNQ)- structure. The reaction of TCNQ with oxidized MnPc yields the ***charge***-transfer complex (TCNQ)δ-·PcMnIII-O-MnIIIPc·(TCNQ)δ-. The Zn and Fe phthalocyanine complexes and the Lu diphthalocyanine complex do not react with TCNQ.
CC 78-3 (Inorganic Chemicals and Reactions)
ST manganese phthalocyanine TCNQ ***charge*** transfer complex
IT Electron exchange and ***Charge*** transfer
(manganese phthalocyanine TCNQ complexes)
IT 174582-02-6 *174582-03-7*

RL: FMU (Formation, unclassified); PRP (Properties); FORM (Formation, nonpreparative)
(formation and absorption spectra of)

IT ***174582-03-7***
RL: FMU (Formation, unclassified); PRP (Properties); FORM (Formation, nonpreparative)
(formation and absorption spectra of)

RN 174582-03-7 ZCAPLUS

CN Manganese, bis[2,2'-(2,5-cyclohexadiene-1,4-diylidene)bis[propanedinitrile]-N]-μ-oxobis[29H,31H-phthalocyaninato(2-)-N29,N30,N31,N32]di- (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

L75 ANSWER 4 OF 9 ZCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1994:148867 ZCAPLUS Full-text
DOCUMENT NUMBER: 120:148867
TITLE: High-photosensitivity electrophotographic photoreceptor
INVENTOR(S): Tai, Seiji; Katayose, Mitsuo; Morishita, Yoshii
PATENT ASSIGNEE(S): Hitachi Chemical Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 22 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 04362653	A	19921215	JP 1991-138909	19910611
PRIORITY APPLN. INFO.:			JP 1991-138909	19910611

GI For diagram(s), see printed CA Issue.

AB In the title electrophotog. photoreceptor comprising an organic photoconductive layer on an elec. conductive support, I [M = Al, Ga, In, Si, Ge, Sn; A1-8 = benzene ring, naphthalene ring, anthracene ring, N-containing aromatic ring; X = halo, R1, OR2, SR3, SiR4R5R6, SO2NR7R8, SO2R9, COR10, COOR11, CONHR12, NR13R14, R15OR16, NO2, SO3H, CN, NHCOR17; g, h, i, j, k, l, m, n = 0-8; Y1,2 = halo, OH, R18, OR19, OSiR20R21R22; R1-22 = H, alkyl, cycloalkyl, aryl, halogenated alkyl, Si-containing group] is utilized as a photoconductive substance in the photoconductive layer. The photoreceptor shows high photosensitivity to the long wavelength region and is suitable for use in a laser printer.

IC ICM G03G005-06

CC 74-3 (Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes)

ST electrophotog photoreceptor ***charge*** generating substance

IT Electrophotographic photoconductors and photoreceptors
(***charge***-generating substances for)

IT 151629-23-1 151629-24-2 151896-69-4 151987-51-8 151987-55-2
151989-12-7 ***151989-13-8*** ***151989-14-9*** 151989-15-0
151989-16-1 151989-18-3 ***151989-19-4*** 151989-20-7
151989-21-8 151989-22-9 151989-23-0 151989-24-1
151989-25-2 152014-43-2 153244-87-2
RL: USES (Uses)
(***charge***-generating material, for electrophotog. photoreceptor)

IT 151627-42-8D, derivs.
RL: USES (Uses)
(***charge***-generating materials, for electrophotog.

photoreceptors)
IT 151627-42-8P 151987-52-9P 151987-53-0P 151987-54-1P 151989-17-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and use of, as ***charge***-generating material, for electrophotog. photoreceptor)
IT 995-25-5, Tri(propyl)chlorosilane 3468-11-9 13134-31-1, 2,3-Diaminopyrazine 19333-10-9, Dichlorosilicon phthalocyanine 82039-07-4, Boron tetrachloride 127009-68-1 151629-11-7 151871-31-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, ***charge***-generating material from, for electrophotog. photoreceptor)
IT ***151989-13-8 151989-14-9 151989-19-4 151989-21-8 151989-25-2***
RL: USES (Uses)
(***charge***-generating material, for electrophotog. photoreceptor)
RN 151989-13-8 ZCAPLUS
CN Gallium, μ-oxobis[C,C,C,C-tetrabromo-29H,31H-phthalocyaninato(2-)-N29,N30,N31,N32]di- (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
RN 151989-14-9 ZCAPLUS
CN Indium, μ-oxobis[C,C,C,C-tetranitro-29H,31H-phthalocyaninato(2-)-N29,N30,N31,N32]di- (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
RN 151989-19-4 ZCAPLUS
CN Germanium, μ-oxobis[29H,31H-phthalocyanine-C,C,C,C-tetrasulfonamidato(2-)-N29,N30,N31,N32]bis(tripropylsilanolato)di- (9CI) (CA INDEX NAME)

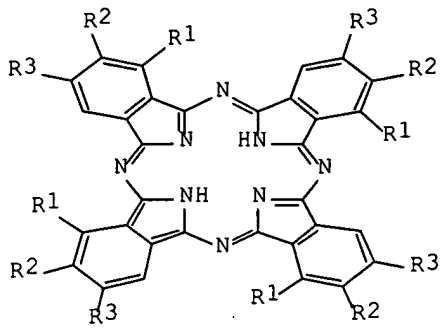
*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
RN 151989-21-8 ZCAPLUS
CN Tin, μ-oxo[C,C,C,C-tetrakis(methylsulfonyl)-29H,31H-phthalocyaninato(2-)-N29,N30,N31,N32][C,C,C,C-tetrakis(methylsulfonyl)-37H,39H-tetranaphtho[2,3-b:2',3'-g:2'',3''-l:2''',3'''-q]porphyrazinato(2-)-N37,N38,N39,N40]bis(tripropylsilanolato)di- (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
RN 151989-25-2 ZCAPLUS
CN Germanium, μ-oxobis[tetramethyl 37H,39H-tetranaphtho[2,3-b:2',3'-g:2'',3''-l:2''',3'''-q]porphyrazine-C,C,C,C-tetracarboxylato(2-)-N37,N38,N39,N40]bis(tripropylsilanolato)di- (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

L75 ANSWER 5 OF 9 ZCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1993:572853 ZCAPLUS Full-text
DOCUMENT NUMBER: 119:172853
TITLE: Phthalocyanines and related compounds. XXXV. Synthesis and coordination chemistry of substituted manganese phthalocyanines
AUTHOR(S): Dolotova, O. V.; Bundina, N. I.; Derkacheva, V. M.; Negrimovskii, V. M.; Minin, V. V.; Larin, G. M.; Kaliya, O. L.; Luk'yanets, E. A.
CORPORATE SOURCE: NII Org. Poluprod. Krasitel., Moscow, Russia
SOURCE: Zhurnal Obshchei Khimii (1992), 62(9), 2064-75
CODEN: ZOKHA4; ISSN: 0044-460X
DOCUMENT TYPE: Journal
LANGUAGE: Russian

GI



I

AB Reaction of substituted phthalonitriles and Mn(OAc)2 in the presence of (NH4)2MoO4 gave MnLX (H2L = I (R1 = R3 = H, R2 = Me3C, PhSO3, Me3CO, Me3CS, piperidine; R2 = R3 = H, R1 = o-ClC6H4, PhSO2, PhS; R2 = H, R3 = Me3C, R1 = PhSO2, PhS, Me2N or R3 = R1 = NO2, PhSO2); X = Cl, OH, OAc). MnLX in pyridine reacted with hot H2O to give [(py)LMn]2O. MnL were obtained by reaction of MnLX with KOH under anaerobic conditions. In pyridine MnL form MnL(py)n (n = 1,2) according to electronic spectra. Their stability toward oxidation-reduction and protolytic conversion depends on the nature of the substituents. Possible electronic isomers of LMnII(py)n (MnIII and MnI ***charge*** transfer compds.) are discussed and these are explained by the energetic nearness of the d-orbitals of Mn and the π-orbitals of L.

CC 78-7 (Inorganic Chemicals and Reactions)
Section cross-reference(s): 26

ST manganese phthalocyaninato complex; ***charge*** transfer manganese phthalocyaninato complex

IT 117778-18-4P 117778-20-8P 117778-21-9P 117778-22-0P 117778-23-1P
117778-24-2P 149785-81-9P 149785-82-0P 149785-83-1P 149785-84-2P
149785-85-3P 149785-86-4P 149785-87-5P 149785-88-6P 149785-89-7P
149785-90-0P 149785-91-1P 149785-92-2P 149785-93-3P 149785-94-4P
149785-95-5P 149785-96-6P 149785-97-7P 149785-98-8P 149785-99-9P
149786-00-5P 149786-01-6P 149786-02-7P 149786-03-8P
149825-79-6P 149825-80-9P 149825-81-0P
149855-30-1P 149855-31-2P 149855-32-3P 149855-33-4P 149855-34-5P
149855-35-6P 149855-36-7P ***149855-37-8P 149855-38-9P***
149855-39-0P 149855-40-3P 149855-41-4P
149855-42-5P 149855-43-6P 149855-44-7P
149855-45-8P 149855-46-9P 149855-47-0P 150120-75-5P
RL: PRP (Properties); PREP (Preparation)
(formation and visible spectrum of)

IT ***149825-82-1P***
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

IT ***149825-79-6P 149825-80-9P 149825-81-0P***
149855-37-8P 149855-38-9P 149855-39-0P
149855-40-3P 149855-41-4P 149855-42-5P
149855-43-6P 149855-44-7P 149855-45-8P
RL: PRP (Properties); PREP (Preparation)
(formation and visible spectrum of)

RN 149825-79-6 ZCAPLUS

CN Manganese, μ-oxobis(pyridine)bis[3,10,17,24-tetrakis(1,1-dimethylethyl)-N,N,N',N',N'',N'',N''',N'''-octamethyl-29H,31H-phthalocyanine-1,8,15,22-tetraminato(2-)-N29,N30,N31,N32]di- (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

RN 149825-80-9 ZCAPLUS

CN Manganese, bis[1,3,8,10,15,17,22,24-octanitro-29H,31H-phthalocyaninato(2-)-N29,N30,N31,N32]-μ-oxobis(pyridine)di- (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

RN 149825-81-0 ZCAPLUS

CN Manganese, bis[1,3,8,10,15,17,22,24-octakis(phenylsulfonyl)-29H,31H-phthalocyaninato(2-)-N29,N30,N31,N32]-μ-oxobis(pyridine)di- (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

RN 149855-37-8 ZCAPLUS

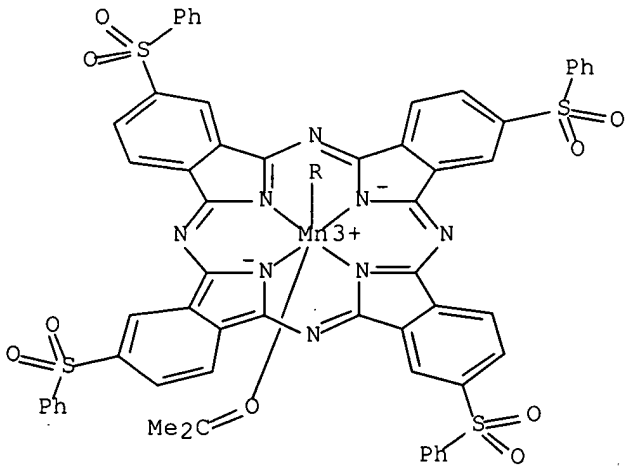
CN Manganese, μ-oxobis(pyridine)bis[2,9,16,23-tetrakis(1,1-dimethylethyl)-29H,31H-phthalocyaninato(2-)-N29,N30,N31,N32]di- (9CI) (CA INDEX NAME)

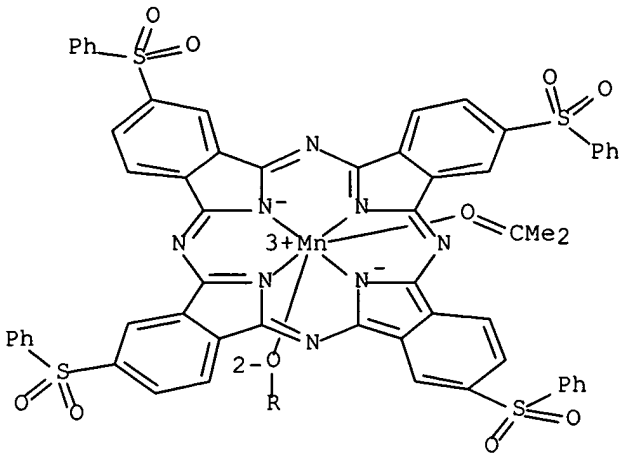
*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

RN 149855-38-9 ZCAPLUS

CN Manganese, μ-oxobis(2-propanone)bis[2,9,16,23-tetrakis(phenylsulfonyl)-29H,31H-phthalocyaninato(2-)-N29,N30,N31,N32]di- (9CI) (CA INDEX NAME)

PAGE 1-A





RN 149855-39-0 ZCAPLUS

CN Manganese, μ-oxobis(pyridine)bis[2,9,16,23-tetrakis(1,1-dimethylethoxy)-29H,31H-phthalocyaninato(2-)-N29,N30,N31,N32]di- (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

RN 149855-40-3 ZCAPLUS

CN Manganese, μ-oxobis(pyridine)bis[2,9,16,23-tetrakis[(1,1-dimethylethyl)thio]-29H,31H-phthalocyaninato(2-)-N29,N30,N31,N32]di- (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

RN 149855-41-4 ZCAPLUS

CN Manganese, μ-oxobis(pyridine)bis[2,9,16,23-tetra-1-piperidinyl-29H,31H-phthalocyaninato(2-)-N29,N30,N31,N32]di- (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

RN 149855-42-5 ZCAPLUS

CN Manganese, μ-oxobis(pyridine)bis[1,8,15,22-tetrakis(phenylsulfonyl)-29H,31H-phthalocyaninato(2-)-N29,N30,N31,N32]di- (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

RN 149855-43-6 ZCAPLUS

CN Manganese, μ-oxobis(pyridine)bis[1,8,15,22-tetrakis(phenylthio)-29H,31H-phthalocyaninato(2-)-N29,N30,N31,N32]di- (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

RN 149855-44-7 ZCAPLUS

CN Manganese, μ-oxobis(pyridine)bis[3,10,17,24-tetrakis(1,1-dimethylethyl)-1,8,15,22-tetrakis(phenylsulfonyl)-29H,31H-phthalocyaninato(2-)-N29,N30,N32,N32]di- (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

RN 149855-45-8 ZCAPLUS

CN Manganese, μ-oxobis(pyridine)bis[3,10,17,24-tetrakis(1,1-dimethylethyl)-1,8,15,22-tetrakis(phenylthio)-29H,31H-phthalocyaninato(2-)-N29,N30,N31,N32]di- (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

IT ***149825-82-1P***
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 149825-82-1 ZCAPLUS
CN Manganese, diaqua-μ-oxobis[2,9,16,23-tetrakis(phenylsulfonyl)-29H,31H-phthalocyaninato(2-)-N29,N30,N31,N32]di- (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

L75 ANSWER 6 OF 9 ZCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1992:70397 ZCAPLUS Full-text
DOCUMENT NUMBER: 116:70397
TITLE: Studies of the adsorption of tetrasulfonated phthalocyanines on graphite substrate
AUTHOR(S): Gupta, S.; Huang, H.; Yeager, E.
CORPORATE SOURCE: Case Cent. Electrochem. Sci., Case West. Reserve Univ., Cleveland, OH, 44106, USA
SOURCE: Electrochimica Acta (1991), 36(14), 2165-9
CODEN: ELCAAV; ISSN: 0013-4686
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The adsorption of iron and cobalt tetrasulfonated phthalocyanines (FeTsPc and CoTsPc, resp.) on ordinary pyrolytic graphite was investigated as a function of pH and ionic strength of the adsorption solution as well as the potential. The ***charge*** corresponding to the voltammetric redox peaks of adsorbed complexes was used as a measure of the surface concentration Adsorption of CoTsPc occurs readily from its freshly prepared aqueous solns. and is generally independent of pH. For FeTsPc, however, adsorption does strongly depend on pH. High surface coverage is achieved only from acid solns. rather than from pure water and alkaline solns. This can be explained in terms of the form(s) fo the complexes existing in the solution phase in the presence of air. UV-visible spectroscopic studies coupled with the addition of CN- to the macrocycle solns. provide evidence that in pure water and alkaline solns. FeTsPc exists predominantly in the μ-oxo form (FeTsPc)2O, which seems not to favor the adsorption process. No evidence of the μ-oxo complex was found for FeTsPc in acid solns. and CoTsPc in aqueous solns. over the pH range examined (1-13). The adsorption of FeTsPc was at maximum when the potential was held at -0.55 V vs. SCE in 0.1M NaOH.
CC 72-2 (Electrochemistry)
Section cross-reference(s): 66, 67
IT ***138708-72-2P***
RL: FORM (Formation, nonpreparative); PREP (Preparation)
(formation of, from monomer in alkaline solns., adsorption of monomer by graphite electrode in relation to)
IT ***138708-72-2P***
RL: FORM (Formation, nonpreparative); PREP (Preparation)
(formation of, from monomer in alkaline solns., adsorption of monomer by graphite electrode in relation to)
RN 138708-72-2 ZCAPLUS
CN Ferrate(8-), μ-oxobis[29H,31H-phthalocyanine-2,9,16,23-tetrasulfonato(6-)-N29,N30,N31,N32]di-, octahydrogen (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

L75 ANSWER 7 OF 9 ZCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1985:122955 ZCAPLUS Full-text
DOCUMENT NUMBER: 102:122955
TITLE: ***Charge***-transfer and ligand-centered photochemistry of manganese(III) phthalocyanines

AUTHOR(S): Ferraudi, G.; Granifo, J.
CORPORATE SOURCE: Radiat. Lab., Univ. Notre Dame, Notre Dame, IN, 46556, USA
SOURCE: Journal of Physical Chemistry (1985), 89(7), 1206-10
CODEN: JPCHAX; ISSN: 0022-3654
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The UV photochem. of the Mn phthalocyanines, MnIII(tspc)(OH2)(OH)4- and (H2O)(tspc)MnIII-O-MnIII(tspc)(OH)9- (tspc = tetrasulfophthalocyanine) was investigated by continuous and flash photolysis. A significant ***charge***-transfer photochem., namely, oxidation of the hydroxide or μ-oxo bridge and the reduction of the metal center was found with both complexes. In addition, the abstraction of H from appropriate donors by phthalocyanine centered nπ* states was also detected. The fate of the Mn(II) species depends on the scavenger used for trapping HO· radicals or reactive nπ* states. So reactions of the 2-hydroxy-2-Pr, hydroxycyclohexadienyl, and hydroxycyclohexadienylsulfonate radicals with either Mn(II) or Mn(III) phthalocyanines determine the nature of the reaction products. The dependence of the rate of the μ-oxo dimer photodissocn. on light intensity demonstrated that recombination of the reduced and oxidized species limited the extent of the conversion to products. The relationship between the photochem. of the Mn(III) phthalocyanines and other metallophthalocyanines is discussed.

CC 74-1 (Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes)

ST manganese phthalocyanine ***charge*** transfer photochem; photolysis manganese sulfophthalocyanine

IT ***12581-70-3***
RL: RCT (Reactant); RACT (Reactant or reagent)
(photochem. of, ***charge***-transfer and ligand centered)

IT 27288-51-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(photochem. of, ***charge***-transfer and ligand-centered)

IT ***12581-70-3***
RL: RCT (Reactant); RACT (Reactant or reagent)
(photochem. of, ***charge***-transfer and ligand centered)

RN 12581-70-3 ZCAPLUS

CN Manganate(9-), aquahydroxy-μ-oxobis[29H,31H-phthalocyanine-C,C,C,C-tetrasulfonato(6-)-N29,N30,N31,N32]di- (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

L75 ANSWER 8 OF 9 ZCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1976:83524 ZCAPLUS Full-text
DOCUMENT NUMBER: 84:83524
ORIGINAL REFERENCE NO.: 84:13619a,13622a
TITLE: Structure and properties of binuclear cobalt(IV) phthalocyanine complexes
AUTHOR(S): Przywarska-Boniecka, Helena; Wojciechowski, Walter
CORPORATE SOURCE: Inst. Chem., Univ. Wroclaw, Wroclaw, Pol.
SOURCE: Materials Science (1975), 1(1), 27-35
CODEN: MSCJDS; ISSN: 0137-1339
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The complexes [{Co(H2O)Pc}2O]SO4, [{Co(OH)Pc}2O], [{Co(NH3)Pc}NH2{Co(H2O)Pc}]Cl3, [{Co(NH3)Pc}NH2{Co(NO3)Pc}]SO4, [{Co(NH3)Pc}O{Co(OH)Pc}]Cl, and [{CoL(H2O)}OH{CoL(OH)}]SO4, where H2Pc = phthalocyanine and H2L = tetrasodium phthalocyaninetetrasulfonate, were prepared and characterized by magnetic susceptibility measurements and ESR, ir and electronic spectra.

CC 78-7 (Inorganic Chemicals and Reactions)
IT 57756-66-8P 57756-67-9P 57756-69-1P ***57756-73-7P***
58098-47-8P 58343-92-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
IT ***57756-73-7P***
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 57756-73-7 ZCAPLUS
CN Cobaltate(6-), aqua-μ-hydroxyhydroxybis[29H,31H-phthalocyanine-C,C,C,C-tetrasulfonato(6-)-N29,N30,N31,N32]di-, sodium sulfate (1:8:1) (9CI) (CA INDEX NAME)

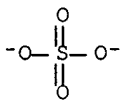
CM 1

CRN 57756-72-6
CMF C64 H28 Co2 N16 O27 S8
CCI CCS, IDS

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

CM 2

CRN 14808-79-8
CMF O4 S



L75 ANSWER 9 OF 9 ZCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1976:11261 ZCAPLUS Full-text
DOCUMENT NUMBER: 84:11261
ORIGINAL REFERENCE NO.: 84:1801a,1804a
TITLE: Electric properties of some cobalt, chromium, and manganese phthalocyanine complexes
AUTHOR(S): Makles, Monika; Przywarska-Boniecka, Helena; Wojciechowski, Walter
CORPORATE SOURCE: Inst. Chem., Univ. Wroclaw, Wroclaw, Pol.
SOURCE: Roczniki Chemii (1975), 49(10), 1647-53
CODEN: ROCHAC; ISSN: 0035-7677
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The elec. properties of 10 phthalocyanine compds. with Co, Cr, and Mn were studied at 160-330°K. From elec.-conductivity measurements of polycryst. samples of the complexes as a function of temperature, the activation energies of conductivity were determined Decreases of activation energy at certain temps. indicated structural changes of the compds. In those regions, ionic conductivity was observed Low activation energies of the complexes containing ions in the outer spheres may be accounted for by the contribution of the ions in the conductivity mechanism. The bridge character of the complexes also contributed to their elec. conductivity
CC 76-2 (Electric Phenomena)

IT 14325-24-7 39368-58-6 57756-65-7 57756-66-8 57756-67-9
57756-69-1 57756-70-4 57756-71-5 ***57756-73-7*** 58098-47-8
RL: PRP (Properties)
(elec. conductivity of)

IT ***57756-73-7***
RL: PRP (Properties)
(elec. conductivity of)

RN 57756-73-7 ZCAPLUS

CN Cobaltate(6-), aqua-μ-hydroxyhydroxybis[29H,31H-phthalocyanine-C,C,C,C-tetrasulfonato(6-)-N29,N30,N31,N32]di-, sodium sulfate (1:8:1) (9CI) (CA INDEX NAME)

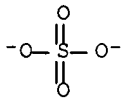
CM 1

CRN 57756-72-6
CMF C64 H28 Co2 N16 O27 S8
CCI CCS, IDS

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

CM 2

CRN 14808-79-8
CMF O4 S



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=>  d his full

     (FILE 'HOME' ENTERED AT 07:55:03 ON 07 DEC 2007)

     FILE 'REGISTRY' ENTERED AT 07:57:31 ON 07 DEC 2007
                ACT WAR884RNS/A
                ---------
L1            21 SEA ABB=ON  PLU=ON  (123833-60-3/BI OR 13450-90-3/BI OR
                  13478-18-7/BI OR 13930-88-6/BI OR 14154-42-8/BI OR 15746-68-6/B
                  I OR 168216-37-3/BI OR 19717-79-4/BI OR 26201-32-1/BI OR
                  634179-07-0/BI OR 634179-08-1/BI OR 634179-09-2/BI OR 634179-10
                  -5/BI OR 634179-11-6/BI OR 634179-46-7/BI OR 634179-47-8/BI OR
                  634179-48-9/BI OR 7446-70-0/BI OR 7550-45-0/BI OR 7718-98-1/BI
                  OR 91-15-6/BI)
                ---------
                ACT WAR884RNS/A
                ---------
L*** DEL      21 SEA FILE=REGISTRY ABB=ON  PLU=ON  (123833-60-3/BI OR 13450-90-3
                ---------
                ACT WAR884HITRNS/A
                ---------
L2  (         21)SEA ABB=ON  PLU=ON  (123833-60-3/BI OR 13450-90-3/BI OR
                  13478-18-7/BI OR 13930-88-6/BI OR 14154-42-8/BI OR 15746-68-6/B
                  I OR 168216-37-3/BI OR 19717-79-4/BI OR 26201-32-1/BI OR
                  634179-07-0/BI OR 634179-08-1/BI OR 634179-09-2/BI OR 634179-10
                  -5/BI OR 634179-11-6/BI OR 634179-46-7/BI OR 634179-47-8/BI OR
                  634179-48-9/BI OR 7446-70-0/BI OR 7550-45-0/BI OR 7718-98-1/BI
                  OR 91-15-6/BI)
L3             7 SEA ABB=ON  PLU=ON  L2 AND NRS>1
                ---------
                ACT WAR884STR20L/A
                ---------
L4               STR
L5          2661 SEA SSS FUL L4
                ---------
                ACT WAR884STR27L/A
                ---------
L6               STR
L7  (       2661)SEA SSS FUL L6
L8               STR
L9           227 SEA SUB=L7 SSS FUL L8
                ---------
                ACT WAR884STR40L/A
                ---------
L10              STR
L11 (       2661)SEA SSS FUL L10
L12              STR
L13          206 SEA SUB=L11 SSS FUL L12
                ---------

     FILE 'ZCAPLUS' ENTERED AT 08:04:54 ON 07 DEC 2007
L*** DEL    3080 S L!3
L14          157 SEA ABB=ON  PLU=ON  L13

     FILE 'REGISTRY' ENTERED AT 08:43:31 ON 07 DEC 2007
L15              STRUCTURE UPLOADED
L16            6 SEA SUB=L5 SSS SAM L15
L17           58 SEA SUB=L5 SSS FUL L15
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                SAVE TEMP WAR884STR15B/A L17

     FILE 'ZCAPLUS' ENTERED AT 08:45:14 ON 07 DEC 2007
L18           50 SEA ABB=ON  PLU=ON  L17

     FILE 'REGISTRY' ENTERED AT 08:45:34 ON 07 DEC 2007
                D SCA L17
L19            6 SEA ABB=ON  PLU=ON  L17 AND ?SULFONYL?/CNS
                D SCA
L20           52 SEA ABB=ON  PLU=ON  L17 NOT L19
L21            0 SEA ABB=ON  PLU=ON  L20 AND L3
                D SCA L3

     FILE 'ZCAPLUS' ENTERED AT 08:59:29 ON 07 DEC 2007
L22           50 SEA ABB=ON  PLU=ON  L20

     FILE 'REGISTRY' ENTERED AT 09:00:52 ON 07 DEC 2007
L23             STRUCTURE UPLOADED
L24             STRUCTURE UPLOADED
L25            9 SEA SUB=L5 SSS SAM L24
L26             STRUCTURE UPLOADED
L27             STRUCTURE UPLOADED
L28             STRUCTURE UPLOADED
L29            9 SEA SUB=L5 SSS SAM L28
L30          111 SEA SUB=L5 SSS FUL L28
L31            0 SEA ABB=ON  PLU=ON  L3 AND L30
L32             STRUCTURE UPLOADED
L33            9 SEA SUB=L5 SSS SAM L32
L34          154 SEA SUB=L5 SSS FUL L32
L35            2 SEA ABB=ON  PLU=ON  L34 AND L3
                D SCA
                D SCA
L36            8 SEA ABB=ON  PLU=ON  L17 AND NC>1
                D SCA
L37            1 SEA ABB=ON  PLU=ON  L36 AND HYDROXIDE/CNS

     FILE 'ZCAPLUS' ENTERED AT 09:24:26 ON 07 DEC 2007
L38            1 SEA ABB=ON  PLU=ON  L37
                D BIB
L*** DEL       0 S L34 AND NC>1

     FILE 'REGISTRY' ENTERED AT 09:25:14 ON 07 DEC 2007
L39           39 SEA ABB=ON  PLU=ON  L34 AND NC>1
                D SCA

     FILE 'STNGUIDE' ENTERED AT 09:30:54 ON 07 DEC 2007

     FILE 'REGISTRY' ENTERED AT 09:39:09 ON 07 DEC 2007

     FILE 'STNGUIDE' ENTERED AT 09:42:34 ON 07 DEC 2007

     FILE 'REGISTRY' ENTERED AT 09:47:20 ON 07 DEC 2007
L40            1 SEA ABB=ON  PLU=ON  L17 AND HYDROXIDE/CNS
L41            6 SEA ABB=ON  PLU=ON  L34 AND HYDROXIDE/CNS
L42            1 SEA ABB=ON  PLU=ON  L34 AND SULFATE/CNS
                D SCA
L43            0 SEA ABB=ON  PLU=ON  L17 AND SULFATE/CNS
L44          154 SEA ABB=ON  PLU=ON  L17 OR L34
L45            1 SEA ABB=ON  PLU=ON  L44 AND CHLORIDE/CNS
                D SCA
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L46             7 SEA ABB=ON  PLU=ON  (L40 OR L41 OR L42)
L47             2 SEA ABB=ON  PLU=ON  L46 AND L3
L48             5 SEA ABB=ON  PLU=ON  L46 NOT L47
                  D SCA

     FILE 'ZCAPLUS' ENTERED AT 09:52:26 ON 07 DEC 2007
L49             4 SEA ABB=ON  PLU=ON  L48
                  D IBIB HITSTR L49 1-4
L50             5 SEA ABB=ON  PLU=ON  L46

     FILE 'REGISTRY' ENTERED AT 09:55:05 ON 07 DEC 2007
                  SEL RN L46
                  SEL CRN L46
L51             8 SEA ABB=ON  PLU=ON  (14808-79-8/RN OR 57756-72-6/RN OR
                  753449-37-5/RN OR 763925-00-4/RN OR 788155-69-1/RN OR 878378-54
                  -2/RN OR 878378-55-3/RN OR 878378-56-4/RN)
                  D SCA
L52             1 SEA ABB=ON  PLU=ON  SULFATE/CN
L53             7 SEA ABB=ON  PLU=ON  L51 NOT L52

     FILE 'ZCAPLUS' ENTERED AT 09:56:35 ON 07 DEC 2007
L54             0 SEA ABB=ON  PLU=ON  L53

     FILE 'REGISTRY' ENTERED AT 09:57:38 ON 07 DEC 2007
L55         17925 SEA ABB=ON  PLU=ON  TETRAKIS/CNS (200W) TETRAKIS/CNS
L56             9 SEA ABB=ON  PLU=ON  L55 AND L34
                  D SCA
L57             1 SEA ABB=ON  PLU=ON  HYDROXIDE/CN
L58             1 SEA ABB=ON  PLU=ON  SULFATE/CN
L59             1 SEA ABB=ON  PLU=ON  CHLORIDE/CN
L60             0 SEA ABB=ON  PLU=ON  H S O/ELF
L61         30961 SEA ABB=ON  PLU=ON  H O S/ELF
L62         30964 SEA ABB=ON  PLU=ON  (L57 OR L58 OR L59 OR L60 OR L61)

     FILE 'ZCAPLUS' ENTERED AT 10:01:32 ON 07 DEC 2007
L63            83 SEA ABB=ON  PLU=ON  L44
L64            50 SEA ABB=ON  PLU=ON  L17
L65             4 SEA ABB=ON  PLU=ON  L62 AND (L63 OR L64)
L66             4 SEA ABB=ON  PLU=ON  L65 NOT L50
                  D SCA
L67             1 SEA ABB=ON  PLU=ON  L66 AND SULFATE/OBI
L68        581403 SEA ABB=ON  PLU=ON  CHARGE/BI
L69             8 SEA ABB=ON  PLU=ON  (L63 OR L64) AND L68
                  D SCA
L70           362 SEA ABB=ON  PLU=ON  TAKAKI K?/AU
L71           929 SEA ABB=ON  PLU=ON  YAMASAKI Y?/AU
L72             7 SEA ABB=ON  PLU=ON  L70 AND L71
L73             3 SEA ABB=ON  PLU=ON  (L70 OR L71) AND (L38 OR L50 OR L67 OR
                  L69)

     FILE 'REGISTRY' ENTERED AT 10:07:20 ON 07 DEC 2007

     FILE 'ZCAPLUS' ENTERED AT 10:07:24 ON 07 DEC 2007
                  D STAT QUE L72
                  D STAT QUE L73
L74             7 SEA ABB=ON  PLU=ON  L72 OR L73
                  D IBIB ABS HITIND HITSTR L74 1-7

     FILE 'REGISTRY' ENTERED AT 10:08:40 ON 07 DEC 2007
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     FILE 'ZCAPLUS' ENTERED AT 10:08:44 ON 07 DEC 2007
                D STAT QUE L38
                D STAT QUE L50
                D STAT QUE L67
                D STAT QUE L69
L75             9 SEA ABB=ON  PLU=ON  (L38 OR L50 OR L67 OR L69) NOT (L72 OR
                  L73)
                D IBIB ABS HITIND HITSTR L75 1-9


     FILE HOME

     FILE REGISTRY
     Property values tagged with IC are from the ZIC/VINITI data file
     provided by InfoChem.

     STRUCTURE FILE UPDATES:    6 DEC 2007  HIGHEST RN 957014-20-9
     DICTIONARY FILE UPDATES:   6 DEC 2007  HIGHEST RN 957014-20-9

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     http://www.cas.org/support/stngen/stndoc/properties.html

     FILE ZCAPLUS

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     FILE LAST UPDATED: 6 Dec 2007  (20071206/ED)

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       This file contains CAS Registry Numbers for easy and accurate
       substance identification.

     FILE STNGUIDE
     FILE CONTAINS CURRENT INFORMATION.
     LAST RELOADED: Nov 30, 2007 (20071130/UP).

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